SPECTRUM

User's Guide

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Processing Data

Processing Data

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

Difference

Derivative

Convert X

Interpolate

Normalization

Absorbance

Transmittance

Baseline Correction

Smooth

Data Tune-up

Arithmetic

Interactive Baseline Correction

Peak Area/Height

ATR Correction

Kubelka–Munk

Deconvolution

Kramers–Kronig

Compare, available on the Process bar by default, requires you to set up compare options and reference spectra.

Peak Table

Biodiesel, available on the Process bar by default, requires you to choose between the standards ASTM D7371 and EN 14078 for the determination of FAME by IR, select Quant methods and parameters and reporting and output settings.

Search, available on the Process bar by default, requires you to set up spectral libraries and search parameters.

MultiSearch, available only if you have the appropriate license for this feature.

Verify, available on the Process bar when a method is available, requires you to add a Verify method to the setup tab.

Quant, available on the Process bar by default.

Adulterant Screen, available only if you have the appropriate license for this feature.

Equations, available on the Process bar by default, requires you to set up one or more equations.

Macros, available on the Process bar by default, requires you to set up one or more Macros.

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

To invoke a process command:

- Select the appropriate command from the Process menu.

  OR

  Click the appropriate icon in the Process bar.

  OR

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

Absorbance

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

1. Display and select the spectrum or spectra that you want to transform to absorbance (A) units.
2. Select **Absorbance** from the Process menu, or click [A icon] on the Process bar.

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

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

Additional Information

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

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

Transmittance

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

1. Display and select the spectrum or spectra that you want to transform to transmittance (%T) units.
2. Select **Transmittance** from the Process menu, or click on the Process bar.

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

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

Additional Information

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

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

Data Tune-up

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

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

1. Display and select the spectrum or spectra that you want to process.
2. Select **Data Tune-up** from the Process menu, or click on the Process bar.
3. The processed spectra are added to the Samples View and displayed in the Viewing Area.

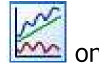
Additional Information

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

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

Baseline Correction

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

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

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

Additional Information

You can use the Baseline Correction process to remove slopes in the baseline of your spectra. Slopes are often caused by scattering of the infrared beam by your sample.

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

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

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

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

Interactive Baseline Correction

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

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

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

   OR

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

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

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

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

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

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

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

   The base point is removed from the baseline.
7. Repeat steps 2 and 3 to identify as many base points as you require.

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

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

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

   In Spectrum ES, Overwrite is not available.

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

   The Baseline Correction dialog closes.

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

   If the Overwrite check box was selected, the processed Source spectrum replaces the source spectrum in the Samples View and is displayed in the Viewing Area.

   Processed spectra are not saved to disk automatically.

Additional Information

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

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

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

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

Difference

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

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

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

   The calculation is always performed in Absorbance.

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

   OR

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

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

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

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

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

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

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

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

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

   OR

   Click **Auto**.

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

   In Spectrum ES, Overwrite is not available.

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

   This dialog is closed.

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

   If the **Overwrite** check box was selected, the difference spectrum replaces the source spectrum in the Samples View and is displayed in the Viewing Area.

   Processed spectra are not saved to disk automatically.

Additional Information

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

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

The difference spectrum is calculated and displayed for the range of data that exists in both source spectra. For example, if one source spectrum has a range of 4400 cm^{-1} to 600 cm^{-1} and the other from 4000 cm^{-1} to 400 cm^{-1}, the resultant difference spectrum will be from 4000 cm^{-1} to 600 cm^{-1}.

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

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

Mixture Search

For information on using the Difference process as part of a Mixture Search, see Search.

Auto-Subtract Spectrum

If you have a Raman instrument, as well as using the Difference command you can also select to Auto-Subtract a spectrum from all spectra immediately after the scan. The raw data is not saved.

Normalization

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

1. Display and select the spectrum or spectra that you want to normalize.
2. Select **Normalization** from the Process menu.

   OR

   Click on the Process bar.

   The Normalization dialog is displayed in the Viewing Area. This dialog contains interactive controls below a **Split** view; the upper graph display contains the selected source spectra, and the lower graph display contains the converted spectra.

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

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

   If **Link graph ranges** is selected, changing the ordinate range displayed in one graph will also change the display of the other.
3. In **Normalize ordinate to**, enter the value, or height, that the common peak should be normalized to.
4. Select the **Abscissa Position** where the common peak can be found in your source spectra.

   By default, the **Maximum ordinate value in the spectrum** of your spectra is selected.

   If you want to normalize your source spectra to a particular peak, click **Maximum ordinate value over defined range**, and then enter (or drag the vertical cursor in the source graph to) a **Start** value to the left, and an **End** value to the right, of the common peak.

   OR

   If you want to normalize your source spectra to an intensity at a particular wavenumber or wavelength, click **Defined position**, and then enter (or drag the vertical cursor in the source graph to) the appropriate value.
5. Select the **Zero Point** for the baseline of your normalized spectra.

   By default, the **Minimum ordinate value** found in your source spectra is set to zero in the normalized spectra.

   If you don't want a baseline correction applied, click **none.**

   OR

   If you want to zero your normalized spectra to the abscissa value at a particular wavenumber or wavelength, click **Selected abscissa point**, and then enter (or drag the vertical cursor in the source graph to) the appropriate value.
6. Select **Overwrite** if you want to overwrite the source spectrum with the corrected spectrum.

   In Spectrum ES, Overwrite is not available.
7. Click **OK** to accept the result.

   This dialog is closed.

If the Overwrite check box was not selected, the normalized spectra are added to the Samples View and displayed in the Viewing pane.

If the Overwrite check box was selected, the normalized spectra replace the selected spectra in the Samples View and are displayed in the Viewing Area

Processed spectra are not saved to disk automatically.

Additional Information

The Normalization process multiplies the ordinate value of each data point in a spectrum by a factor that scales a particular peak to a set limit. This enables you to compare the spectrum with spectra that include the same peak scaled to the same limit. All %T calculations are performed internally in Absorbance, to minimize any affect on the shape of the peaks.

Normalization is particularly important when comparing Raman spectra collected using different instruments. It is also useful when looking at the effect of polarization on Raman spectra.

Interpolation

Use the Interpolation process command to change the number of data points in one or more spectra and, if necessary, their range.

1. Display and select the spectrum or spectra that you want to interpolate.
2. Select **Interpolation** from the Process menu.

   OR

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

   The Interpolation dialog is displayed in the Viewing Area. This dialog contains interactive controls below a **Split** view; the upper graph display contains the selected source spectra, and the lower graph display contains the converted spectra.

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

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

   If **Link graph ranges** is selected, changing the ordinate range displayed in one graph will also change the range of the other.
3. If you want to use part of the **Full range** of your selected source spectra, click **Selected range**, and then enter (or drag the vertical cursor in the source graph to) the **Start** and **End** values for your range of interest.
4. If necessary, enter an appropriate new **Data point interval**.

   The default data interval maintains the number of points in the source spectra.
5. Select **Overwrite** if you want to overwrite the source spectrum with the corrected spectrum.

   In Spectrum ES, Overwrite is not available.
6. Click **OK** to accept the result.

   This dialog is closed.

   If the Overwrite check box was not selected, the interpolated spectra are added to the Samples View and displayed in the Viewing pane.

   If the Overwrite check box was selected, the interpolated spectra replace the selected spectra in the Samples View and are displayed in the Viewing Area.

   Processed spectra are not saved to disk automatically.

Additional Information

Use the Interpolation process command to:

- Save part of a spectrum
- Reduce the number of data points.

  The number of data points in a spectrum is included in the Sample section its History tab.

The Interpolation process adds data points to a spectrum by adding new points between the points that already exist, and removes data points from a spectrum by selecting every nth point in a spectrum and deleting it.

The number of data points needed in a spectrum depends on the width of the features in the spectrum. If the separation of the data points is smaller than is needed to define the features in the spectrum, the number of points can be reduced without reducing the amount of information in the spectrum.

Increasing the number of data points in a spectrum cannot increase the amount of information in the spectrum.

Interpolation can be used to convert your spectra before comparing them with spectra in third-party libraries.

Convert X

Use the ConvertX process command to convert the abscissa units of your infrared spectra to and from wavenumbers, microns, or nanometers. You can also convert Raman data from Raman Shift (cm-1) to absolute wavenumbers (cm-1).

1. Display and select the spectrum or spectra that you want to convert.
2. Select **ConvertX** from the Process menu.

   OR

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

   The ConvertX dialog is displayed in the Viewing Area. This dialog contains interactive controls below a **Split** view; the upper graph display contains the selected source spectra, and the lower graph display contains the converted spectra.

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

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

   If **Link graph ranges** is selected, changing the ordinate range displayed in one graph will also change the display of the other.
3. Select the **New abscissa unit** that you want to convert to.
4. If necessary, enter an appropriate **Data point interval**.

   The current data interval is selected by default. This maintains the number of points in the source spectra.
5. If you want the converted spectra to replace your source spectra, select the **Overwrite** check box.

   In Spectrum ES, Overwrite is not available.
6. Click **OK** to accept the result.

   This dialog is closed.

   If the Overwrite check box was not selected, the converted spectra are added to the Samples View and displayed in the Viewing Area.

   If the Overwrite check box was selected, the converted spectra replace the selected spectra in the Samples View and are displayed in the Viewing Area.

   Processed spectra are not saved to disk automatically.

Additional Information

For most applications in chemistry, mid infrared spectra are displayed on an abscissa scale that is linear in wavenumber. Fourier Transform interferometers generate data points at equally spaced frequency intervals, so a linear wavenumber scale (frequency divided by the speed of light) is natural.

However, for some applications a linear wavelength scale is preferred, measured in microns or nanometers. Near infrared spectra, for example, often have a nanometer abscissa scale. The transformation from a wavenumber scale to a wavelength scale is non-linear.

Data Interval

You can change the data interval of your FT-IR spectrum when you change the abscissa scale.

A direct conversion between scales may be unsatisfactory because it results in an uneven distribution of data points. Convert X uses interpolation to produce spectra with equally-spaced data points. However, if the conversion were to maintain the smallest data interval found in the source spectra, the number of interpolated points can become large.

Smooth

Use the Smooth process command to reduce the noise level in one or more spectra.

CAUTION: Use the Smooth process with discretion. It can remove important data and generate misleading results by reducing the number of data points in the spectrum. Spectra that have plateau regions adjacent to sharp peaks (typical for gas samples, and some NIR and Raman spectra) are especially vulnerable to excessive smoothing.

1. Display and select the spectrum or spectra that you want to smooth.
2. Select **Smooth** from the Process menu, or click on the Process bar.
3. Select the **Smooth Factor** you wish to apply.
4. If you want the smoothed spectra to replace your source spectra, select the **Overwrite** check box.

   In Spectrum ES, Overwrite is not available.
5. Click **OK**.

   This dialog is closed.

   If the Overwrite check box was not selected, the smoothed spectra are added to the Samples View and displayed in the Viewing Area.

   If the Overwrite check box was selected, the smoothed spectra replace the selected spectra in the Samples View and are displayed in the Viewing Area.

Additional Information

Smoothing is a form of filtering that reduces noise, but also degrades the resolution of your spectrum so that the features in the spectrum become broader. If you use too great a level of smoothing, bands are broadened excessively and resolution is lost.

Smoothing should not change band areas or the position of symmetrical bands.

The Smooth process used is an adaptive procedure that estimates the signal-to-noise ratio of the data within a window and then applies an appropriate degree of smoothing. Areas with a high signal-to-noise ratio have no smoothing applied to them, and noisy areas are heavily smoothed.

The window size is appropriate for 4 cm^{-1} resolution data, which means that the smooth algorithm is unsuitable for spectra with very sharp peaks.

Derivative

Use the Derivative process command to generate a first, second, third or fourth order derivative curve from your selected spectrum.

1. Display and select the spectrum, or spectra, that you want to process.
2. Select **Derivative** from the Process menu.

   OR

   Click if you have it available on the Process bar.

   The derivable dialog is displayed in the Viewing Area. This dialog contains interactive controls below a **Split** view; the upper graph display contains the selected source spectra, and the lower graph contains the calculated derivative curves.

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

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

   If **Link graph ranges** is selected, changing the ordinate range displayed in one graph will also change the range of the other.
3. Select the **Order** of the derivative, and the **Number of Points** to provide the required degree of smoothing.
4. If you want the calculated derivative curves to replace your source spectra, select the **Overwrite** check box.

   In Spectrum ES, Overwrite is not available.
5. Click **OK** to accept the result.

   This dialog is closed.

   If the Overwrite check box was not selected, the derivative curves are added to the Samples View and are displayed in the Viewing Area.

   If the Overwrite check box was selected, the derivative curves replace the selected spectra in the Samples View and are displayed in the Viewing Area.

   Processed spectra are not saved to disk automatically.

Additional Information

Derivative curves usually have sharper features than the original spectra, which can enable you to reduce the effects of overlapping bands and to suppress background effects. You can use derivative curves in quantitative methods to eliminate some baseline effects. For example, the amplitudes of features in derivative curves can be used in the same way as peak absorbances.

Order

The first derivative removes any baseline offset and linear slope.

The second derivative removes any parabolic baseline effects. These curves have sharp minima where there are maxima in the original spectrum, which can enable you to identify band positions in complex regions.

The third derivative removes any cubic baseline effects, and the fourth derivative any fourth order baseline effects. Both third and fourth order derivative curves can be difficult to interpret, and are only useful when the original spectra had a high signal-to-noise ratio.

Smoothing by varying the number of data points used for the slope calculation

Derivative curves emphasize narrow features, including noise, relative to broad ones. You can control this to some extent by varying the width (that is, the **Number of Points** used to calculate the slope) of the derivative function, which is equivalent to applying some smoothing to the derivative curve.

The Derivative process uses the Savitzky-Golay procedure to estimate the derivative of a smooth curve, constructed through the original data points of your original spectrum. It uses a number of neighboring data points to estimate the curve. As the number of data points used in the calculation is increased, the contribution of broader features increases relative to narrow features.

Raman data

Derivative is particularly useful to correct for spikes in your Raman data, for example, due to cosmic rays. It is also useful for removing baseline slope due to fluorescence.

ATR Correction

ATR Correction is used to make spectra that have been collected with an Attenuated Total Reflection (or Multiple Internal Reflection) accessory similar to transmittance spectra. A corrected spectrum can then be compared with a transmittance spectrum.

The most significant difference between internal reflection spectra and transmittance spectra relates to the relative band intensities. In general, ATR spectra show enhanced band intensities at longer wavelengths. In ATR measurements, the equivalent of pathlength is the effective penetration depth of the radiation into the sample. This penetration depth is proportional to wavelength. The ATR Correction scales the intensities by a factor that is inversely proportional to wavelength, making them more similar to those in transmittance spectra.

ATR correction also enables you to correct for less than perfect contact between your sample and the ATR crystal. If the surface of the sample is not optically flat, there will be an air gap between the crystal and the sample in some places. The effect on band intensities is greater at short wavelengths than at longer wavelengths because the gap represents a greater proportion of the penetration depth. However, the reduction in intensities caused by the gap is not simply proportional to wavelength. The **Contact** function attempts to provide correction for this effect. Because any air gap is not uniform, this second correction term should be regarded as an empirical adjustment.

Using ATR Correction

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

   OR

   Click on the Process bar.

   The ATR Correction dialog is displayed in the Viewing Area.

   This dialog contains interactive controls below a **Split** view; the upper graph display contains the selected source spectra, and the lower graph display contains the converted spectra.

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

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

   If **Link graph ranges** is selected, changing the ordinate range displayed in one graph will also change the range of the other.
3. In **Contact**, enter a contact correction factor, if necessary.

   Enter a value between 0 and 2.2.

   For perfect contact, the penetration depth is proportional to the wavelength and the contact factor is 0.
4. Select **Overwrite** if you want to overwrite the source spectrum with the corrected spectrum.

   In Spectrum ES, Overwrite is not available.
5. Click **OK** to accept the result.

   This dialog is closed.

If the Overwrite check box was not selected, the corrected spectra are added to the Samples View and displayed in the Viewing pane.

If the Overwrite check box was selected, the corrected spectra replace the selected spectra in the Samples View and are displayed in the Viewing Area.

Processed spectra are not saved to disk automatically.

Additional Information

ATR spectra also differ from transmittance spectra in band shape and positions. These differences should be remembered when comparing ATR and transmittance spectra.

Arithmetic

Use the Arithmetic process command to apply one or more of the following operations to your spectra:

+	addition	requires an operand
-	subtraction	requires an operand
x	multiplication	requires an operand
/	division	requires an operand
log	log base 10	
ln	log base e	
sqr	square	
sqrt	square root	

For example, you could multiply the ordinate values in a spectrum by a constant (such as 2), or divide one spectrum by another spectrum.

1. Display and select the spectrum that you want to process.
2. Select **Arithmetic** from the Process menu.

   OR

   Click + − ÷ × if you have made it available on the Process bar.

   The arithmetic dialog is displayed in the Viewing Area. This dialog contains interactive controls below a **Split** view; the upper graph display contains the selected source spectrum, and the lower graph display will contain the processed spectrum.

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

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

   If **Link graph ranges** is selected, changing the ordinate range displayed in one graph will also change the range of the other.
3. Select the **Operator** you require from the drop-down list
4. Enter the value of the **Constant** to apply to your spectrum.

   For example, **Current Sample x 2** multiplies the ordinate values in your spectrum by 2.

   OR (and provided you selected the +, -, x or / operator)

   Deselect the **Constant** button, and then select another spectrum from the **Operand** drop-down list; the browse option enables you to select any *.sp file available to your PC.

   The operation is performed and the **Arithmetic Result** graph display is updated.

NOTE: If you select **log**, **ln**, **sqr**, or **sqrt** the **Operand** field is not available because no other spectrum is required to complete these operations.

OR

If the sample table contains a File Path custom column, click the **Column** button and select the name of the custom column from the drop-down list.

The operation is performed on the sample using the spectrum file in the custom column of the sample table.

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

   In Spectrum ES, Overwrite is not available.

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

   This dialog is closed.

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

   If the Overwrite check box was selected, the processed spectra replace the selected spectra in the Samples View and are displayed in the Viewing Area.

   In Spectrum ES, Overwrite is not available.

   Processed spectra are not saved to disk automatically.

Additional Information

Negative values in the logarithmic and square root operations

For logarithmic and square root operations, negative input values are set to zero.

Spectra that have different units

When you add or subtract two spectra, the ordinate axis of the resulting spectrum has the units of the first spectrum.

When you multiply or divide two spectra, the values in the resulting spectrum are multiplied or divided by 100 (as appropriate) and the units of the ordinate axis change:

Units of Spectrum 1	Units of Spectrum 2	Operation	Post-Treatment	Units of Result
Any	%T	divide	x100	Units of Spectrum 1
Any	%R	divide	x100	Units of Spectrum 1
Egy	Egy	divide	x100	%T
%T	%T	multiply	/100	%T
%T	%R	multiply	/100	Arbitrary
%R	%T	multiply	/100	Arbitrary
%R	%R	multiply	/100	%R

NOTE: Dividing (ratioing) two energy spectra produces a spectrum in %T.

Adding Spectra

If you add two spectra with the same units and the same range but with different data intervals, the resulting spectrum is constructed using the smaller data interval.

If you add two spectra with the same units and data intervals but with different ranges, the resulting spectrum is the sum of the overlapping regions only.

Subtracting Spectra

If you subtract two spectra with the same units and range but different data intervals, the resulting spectrum is constructed using the smaller data interval.

If you subtract two spectra with the same units and data intervals but different ranges, the resulting spectrum is the difference of the overlapping regions only.

Multiplying Spectra

If you multiply two spectra with the same units, data interval and range, the resulting spectrum is the product of the two spectra.

If you multiply two spectra with the same units and ranges but different data intervals, the resulting spectrum is constructed using the smaller data interval.

If you multiply two spectra with the same units and data intervals but different ranges, the resulting spectrum is the product of the overlapping regions only.

Dividing Spectra

If you divide two spectra with the same units, data interval and range, the resulting spectrum is the ratio of the two spectra.

If you divide two spectra with the same units and ranges but different data intervals, the resulting spectrum is the ratio constructed from the smaller data interval.

If you divide two spectra with the units and data intervals but different ranges, the resulting spectrum is the ratio of the overlapping regions only.

Kubelka–Munk

The Kubelka–Munk transform converts a spectrum with reflectance as its ordinate to Kubelka–Munk units.

1. Display and select the diffuse reflectance spectrum or spectra that you wish to convert to K-M units.

   The spectrum shown is in reflectance units.

2. Select **Kubelka–Munk** from the Process menu.

   OR

   Click f(x) KM on the Process bar.

3. Display the Process menu and choose **Kubelka–Munk**.

   The spectrum is displayed in K-M units.

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

NOTE:	Performing the Kubelka–Munk transform on a spectrum that is already in K-M units will convert it to Reflectance units.

Additional Information

This transform is used with the diffuse reflectance spectra of powders. In theory, after Kubelka–Munk transformation, the band intensities vary linearly with concentration (obey Beer's Law). So, you would use Kubelka–Munk for diffuse reflectance spectra just as you would use absorbance for spectra measured in transmittance. You will find most mid infrared diffuse reflectance spectra in the literature presented in K–M units.

However, it has been very difficult to obtain good quantitative results from diffuse reflectance spectra in the mid infrared region. The main reason is that absorption in this region is very strong, whereas the Kubelka–Munk theory is strictly applicable only to very weak absorption.

The Kubelka–Munk command converts a reflectance spectrum, R, to K–M units, using the relationship:

$$F(R) = \frac{(1 - R)^2}{2R}$$

where R is the reflectance spectrum and F(R) is the Kubelka–Munk spectrum.

If the reflectance spectrum has any totally absorbing bands, they are truncated at 0.0655% to avoid division by zero.

Kramers–Kronig

NOTE: This scale is not suitable for diffuse reflectance spectra; for diffuse reflectance spectra you should use Kubelka–Munk as the ordinate scale.

Use the Kramers–Kronig process command to transform one or more spectra whose ordinate scale is in specular reflectance units to spectra whose ordinate scale is in absorbance (A) units.

1. Display and select the spectrum or spectra that you want to transform to absorbance (A) units.
2. Select **Kramers–Kronig** from the Process menu.

   OR

   Click f(x) KK if you have made it available on the Process bar.

   The Kramers–Kronig dialog is displayed in the Viewing Area. This dialog contains interactive controls below a **Split** view; the upper graph display contains the source spectrum, and the lower graph contains the result spectra.

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

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

   If **Link graph ranges** is selected, changing the ordinate range displayed in one graph will also change the range of the other.
3. Enter the **Start** and **End** wavenumber values for your range of interest.
4. In **Calculate/Destination**, select **N-Index** if you wish to generate a refractive index spectrum and/or **K-Index** if you wish to generate an absorption index spectrum.

   NOTE: When using Kramers–Kronig as part of a macro, you can only select Absorbance or K-Index or N-index. To generate a K-Index or N-index when using the Kramers–Kronig transform in a Macro, first create an **Absorbance** process step to generate an absorbance spectrum. Then create a Kramers–Kronig process step and select either **K-Index** or **N-Index**.
5. Select **Overwrite** if you want to overwrite the source spectrum with the converted spectrum.
6. In Spectrum ES, Overwrite is not available.

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

   This dialog is closed.

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

   If the Overwrite check box was selected, the processed Source spectrum replaces the source spectrum in the Samples View and is displayed in the Viewing Area.

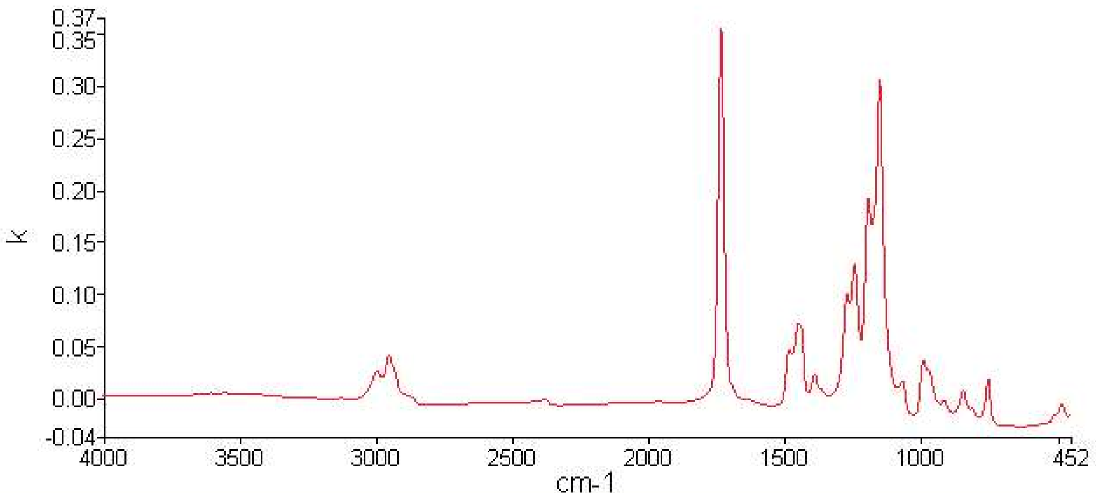
   Processed spectra are not saved to disk automatically.

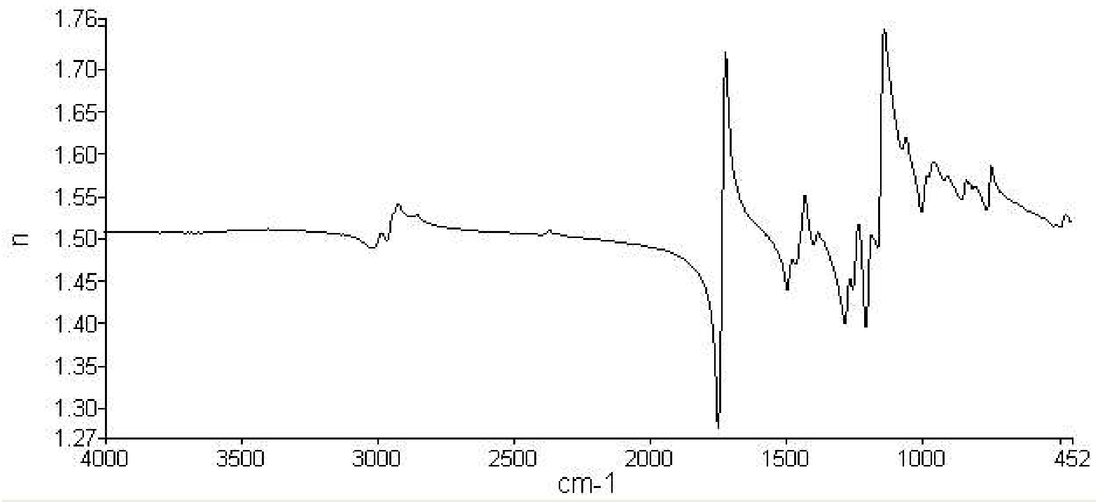
Additional Information

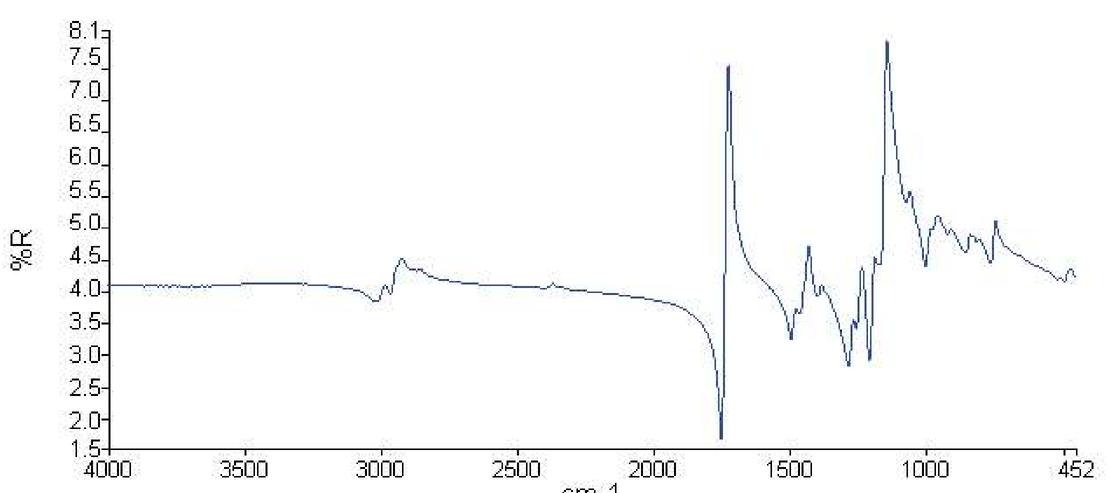
Specular reflectance spectra typically have derivative-like features rather than symmetrical absorption bands. The Kramers–Kronig transform calculates an absorbance spectrum from a specular reflectance spectrum. As most spectra in spectral libraries are collected in transmission, this transform facilitates the identification of spectra using Search. With the Kramers–Kronig transform, you can also display an absorption index and/or a refractive index spectrum calculated from the specular reflectance spectrum. This is because not only does the absorption of a sample change with wavelength, but also its refractive index.

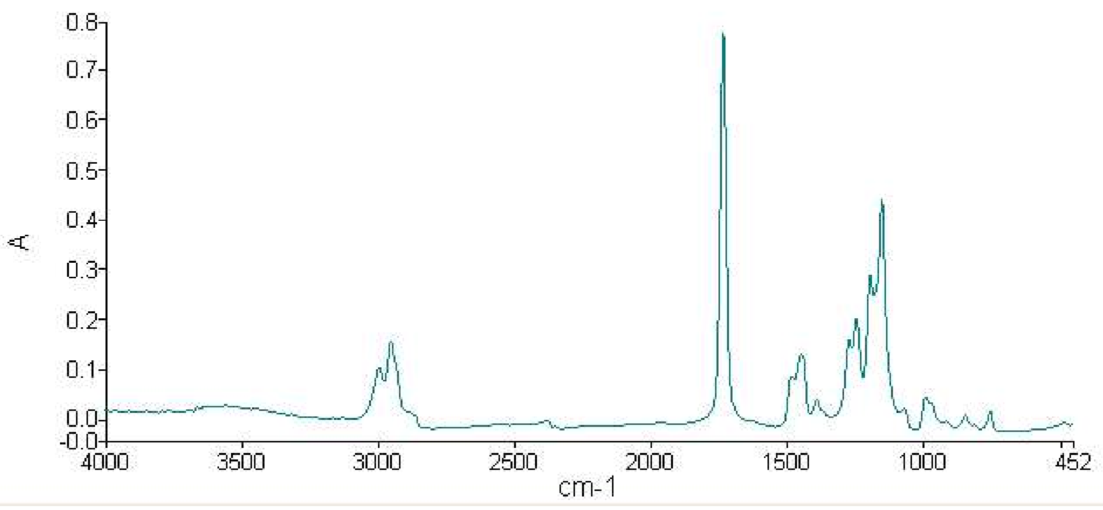
The Kramers–Kronig scale is suitable if your spectrum was collected from a smooth, shiny surface of a uniform sample. It is not applicable to diffuse reflectance spectra. The use of the Kramers–Kronig transform is NOT appropriate for spectra collected in the near infrared.

A typical specular reflectance spectrum and the spectra generated by the transform are shown below:




n
1.76
1.70
1.65
1.60
1.55
1.50
1.45
1.40
1.35
1.30
1.27
4000
3500
3000
2500
2000
1500
1000
452
cm-1


%R
8.1
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
4000
3500
3000
2500
2000
1500
1000
452
cm-1


A
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-0.0
4000
3500
3000
2500
2000
1500
1000
452
cm-1

Very often, reflectance spectra are a mixture of specular and diffuse reflection. The Kramers–Kronig transform may help qualitative interpretation in such spectra if the contribution from surface reflection is dominant, but you will find distorted band shapes and intensities. For best results, there should be baseline regions free from bands at each end of the region of the spectrum that you wish to transform.

NOTE: To view the History, display the History tab. The parameters saved include the abscissa start value of the region processed; the abscissa end value of the region processed; A: absorbance spectrum; K: absorption index spectrum; N: refractive index spectrum.

Deconvolution

Deconvolution applies a line-narrowing process so that interference between unresolved features is reduced. This means that you can see peaks that are present more easily. Deconvolution is used in estimating the positions and intensities of overlapping absorption bands.

1. Display and select the spectrum or spectra that you want to deconvolute.
2. Select **Deconvolution** from the Process menu.

   OR

   Click on the Process bar.

   The Deconvolution dialog is displayed in the Viewing Area. This dialog contains interactive controls below a **Split** view; the upper graph display contains the selected source spectra, and the lower graph display contains the converted spectra.

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

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

   If **Link graph ranges** is selected, changing the ordinate range displayed in one graph will also change the range of the other.
3. Enter the **Gamma** value, which defines the line-narrowing and can take values between 0 and 100; larger values give more narrowing.

   The reduction in linewidth for an ideal Lorentzian line is given by: 4 * Gamma * data interval. For spectra with a data interval of 1, typical gamma values are less than 3.
4. Select the smoothing **Length**.

   Length defines the smoothing that is applied to limit the noise generated by line-narrowing. It can take values between 0 and 95, with 95 corresponding to maximum smoothing.
5. Select the appropriate radio button for either **Bessel** or **Boxcar** smoothing.

   You should choose Bessel for real data.
6. Select **Overwrite** if you want to overwrite the source spectrum with the corrected spectrum.

   In Spectrum ES, Overwrite is not available.
7. Click **OK** to accept the result.

   This dialog is closed.

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

   If the Overwrite check box was selected, the processed Source spectrum replaces the source spectrum in the Samples View and is displayed in the Viewing Area.

   Processed spectra are not saved to disk automatically.

Additional Information

Deconvolution applies a line-narrowing process so that interference between unresolved features is reduced. This has traditionally been done by taking derivatives of the spectrum. For example the second derivative of a band has a narrow minimum at the frequency corresponding to the maximum of the original band. The disadvantage of derivative spectra is that secondary maxima and minima are generated along with the central features. Deconvolution achieves line-narrowing with minimal subsidiary features.

Deconvolution uses a method called Fourier self-deconvolution which operates on the Fourier transform of the spectrum. It can be thought of as involving two steps. A line narrowing filter removes broadening corresponding to a Lorentzian line shape. This filter is characterized by Gamma. Increasing the magnitude of Gamma produces narrower lines, but eventually leads to subsidiary features (sidelobes) around the narrowest bands. It also increases the noise. To reduce these undesired effects a smoothing function is applied. The degree of smoothing is controlled by a parameter called length. Increasing the length leads to a greater degree of smoothing. This reduces noise and sidelobes, but at the expense of some line broadening.

Deconvolution is an interactive routine to find the most appropriate combination of these parameters. It has to be used with caution since sidelobes from large bands can be confused with small overlapping bands.

Deconvolution works best with noise-free data where all the bands are Lorentzian and have the same width. Even with ideal data the line width cannot be reduced below the resolution at which the spectrum was collected. With real data, the degree of narrowing that can be achieved is limited either by noise or by the subsidiary features associated with the sharpest bands.

There is no correct result for real data. For example, small negative sidelobes may be perfectly acceptable when trying to identify band positions.

Biodiesel

The Biodiesel process command enables you to determine the fatty acid methyl esters (FAME) concentration in diesel/biodiesel blends, using either the ASTM D7371 or the EN 14708 standard.

Biodiesel FAME ASTM D7371 uses FT-MIR with an attenuated total reflectance (ATR) sampling accessory. European standard EN 14078 uses FT-MIR with a liquid cell of known pathlength.

Once you have set up Biodiesel, use the process to determine the FAME content of your samples. FAME Vol% will be determined for the spectra selected using the Standard selected on the Biodiesel (FAME) Settings tab.

1. Display and select the spectrum or spectra that you want to process.
2. Select **Biodiesel** from the Process menu.

   OR

   Click the icon on the Process bar.

   The Biodiesel process is performed, and the results are displayed in the Results Table.

Biodiesel FAME ASTM D7371 Results

The **FAME Vol %**, **FAME Residual Ratio** and **FAME Total M-Distance** are displayed by default in the Results Table. You can also choose to display the **FAME RMS Residual** and **FAME P2P Residual**.

The Biodiesel FAME ASTM D7371 results are available in the Equation Variables list on the Setup Equation Properties dialog. They are also added to the analysis report and analysis results file.

When the process is performed, the FAME Vol% is calculated first using the low concentration method. If the result is >10%, the FAME Vol% will be determined using the medium concentration method. If FAME Vol% ≤10.5%, the result determined by the low concentration method will be used. If 10.5% < FAME Vol% ≤ 30%, the value determined by the medium concentration will be used. If 30.5% < FAME Vol% ≤ 100%, the value determined by the high concentration method will be reported, if a high concentration method was selected. If a high concentration method was not selected, the value obtained using the medium concentration method will be used.

The FAME Residual Ratio is the ratio of the residual variance of the unknown to the residual variance of the calibration standards. A high value compared to those seen for independent validation standards suggests that the residual spectrum contains features not modeled during calibration. In such cases, the prediction results should be treated with caution and the features in the residual spectrum investigated.

The FAME Total M-distance ratio is the ratio between the Mahalanobis distance for the unknown sample and the leverage cutoff. The leverage cutoff reflects twice the average leverage of the calibration standards. A value significantly greater than 1 for the Total M-distance ratio may indicate that the unknown sample lies outside the calibration set. In such cases the prediction results must be treated with caution. The Total M-distance ratio may exceed 1 if there are additional overlapping features in the unknown spectrum that have not been modeled, or if the modeled features are more intense than those in the calibration set (extrapolation). The residual ratio enables you to distinguish between these two cases. Additional unmodeled features in the unknown spectrum which do not overlap will not affect the M-distance, but will increase the residual ratio.

The RMS (Root Mean Square) residual is a measure of the average error (standard deviation) associated with the residual spectrum. This value should be comparable to the RMS noise level in the unknown spectrum.

The FAME P2P (Peak to Peak) Residual represents the maximum range of deviation between the original (unknown) spectrum and the calculated spectrum (maximum residual – minimum residual). Typically, this value should be in the order of five times the RMS error if the residuals consist of only random noise. A high value for the FAME P2P (Peak to Peak) Residual can indicate that there are features in the unknown sample that were not present in the calibration set. It is advisable to view the residual spectrum to determine the origin of the unmodeled feature.

See the "Mathematical Discussion" in the Spectrum Quant+ on-screen Help for mathematical definitions of these terms.

Biodiesel EN 14078 Results

The **FAME Vol%** is displayed by default in the Results Table. You can also choose to display the **Pathlength**, **Dilution Factor** and **FAME Error of prediction**.

The Biodiesel EN 14078 results are available in the Equation Variables list on the Setup Equation Properties dialog.

The FAME error of prediction is a standard statistical estimate of the uncertainty associated with the prediction, and is reported as a Vol%.

Additional Information

References

ASTM D7371–07: Standard Test Method for Determination of Biodiesel (Fatty Acid Methyl Esters) Content in Diesel Fuel Oil Using Mid Infrared Spectroscopy (FT-IR-ATR-PLS Method).

EN 14078:2003 Determination of fatty acid methyl esters (FAME) in middle distillates (Infrared spectroscopy method).

Peak Table

Peak Table is a process command that automatically produces a table of the peaks in your spectrum or spectra. The parameters used to generate the Peak Table are defined on the Setup Peak Detection tab.

1. Display and select the spectrum or spectra that you want to process.

   Select **Peak Table** from the Process menu.

   OR

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

The results are displayed on the Peak Table tab in the Viewing Area.

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

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

  To view this table in detail, it may be helpful to drag the borders between the quadrants.
- The List of Peaks for each spectrum is tabulated in the upper right quadrant of the Peak Table tab.

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

  To view this table in detail, it may be helpful to drag the borders between the quadrants.
- Your source spectrum or spectra are displayed in a graph below the results tables with the peak X and Y positions labeled.
- Use the shortcut menu to **Copy** the Peak Table to the clipboard, or use the **Send To** command to copy the contents of the Viewing Area into a Word or WordPad document.

The results are also displayed on the Results Table tab.

Additional Information

The results of the Peak Area/Height process are also added to the Peak Table tab. Each time you run a Peak Table or Peak Area/Height process on a spectrum, a new row is appended to the results.

Peak Area/Height

Peak Area/Height is a process command that enables you to produce a table of the areas and heights of the peaks in your spectrum or spectra. You can auto-generate a peak table, or add peaks individually. You can use it to measure:

- Peak areas relative to a linear baseline, between two baseline points, or between two other points on the spectrum.
- Peak heights from a peak maximum to a baseline.
- The maximum height in a selected region.
- The ratio of two peaks.

You can run the Peak Area/Height process on multiple spectra. However, note that the same parameters will be used to produce the results for all the spectra selected. If you wish to use different parameters for each spectrum, you should process the spectra individually.

1. Display and select the spectrum or spectra that you want to process.
2. Select **Peak Area/Height** from the Process menu.

   OR

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

   The Peak Area/Height dialog is displayed in the Viewing Area.
3. Select the spectrum you would like to display while defining the peaks from the drop-down list.

   If you selected more than one spectrum before selecting Peak Area/Height, those spectra will be available in the drop-down list. Although only one spectrum is displayed, the same parameters will be used to generate the results for all the spectra. If you wish to use different parameters for each spectrum, you will need to process the spectra individually.
4. Select to display the **Area** or **Height** graph marker.
5. In the **Calculation** section, choose whether to calculate **Area**, **Height** or **Max Height**.

   Areas and heights are calculated in the same units as the spectrum. If you want to use units different from the current units of the spectrum, you must convert the spectrum to the correct units first.
6. Select the number of Bases.

   Select **Base 1**, **Base 2**. If one or more bases are selected, then **Min Bases** becomes available.

   If no bases are selected, the zero absorbance is used as the baseline. If Base 1 is selected, a horizontal baseline is drawn at that ordinate value. If Base 1 and Base 2 are selected, the baseline is drawn between the two points.

   Min Bases adds range markers for each base point. The base point used is the minimum value between the markers.

7. Click **Add** to add a peak (defined at the current Vertical Cursor position) to the table.

   OR

   Double click on the Vertical Cursor to add a peak to the table.

   OR

   Click **Auto** to automatically find the peaks and populate the table.

8. Use the graph markers to adjust the position of the baseline markers, the range over which the peak area or maximum height will be calculated, or the point on the curve at which the height will be determined, as required.

9. Select the results you want to be displayed in the Results Table.

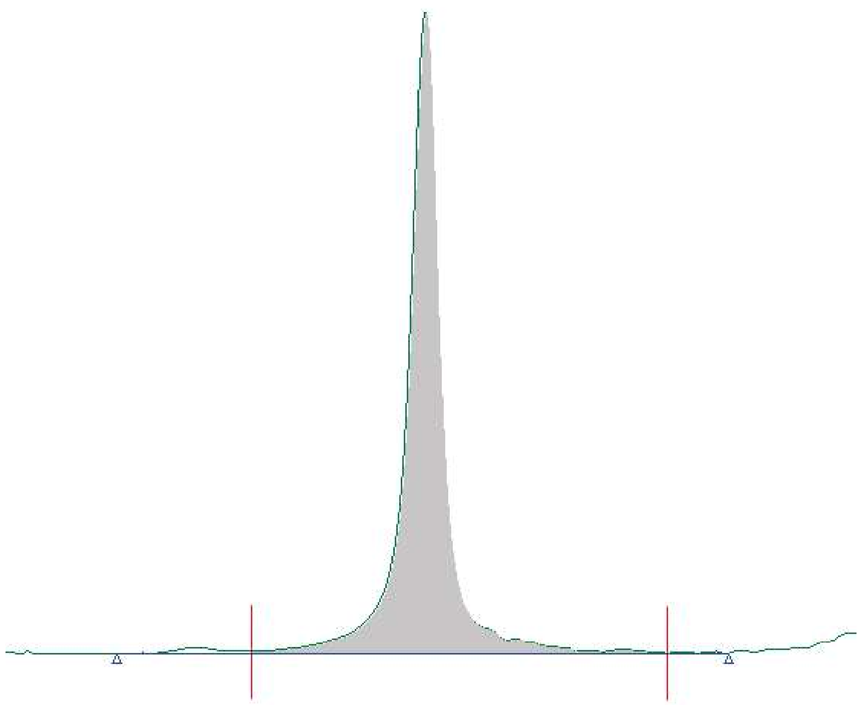
   The options are the **X** and/or **Y** coordinates, **Height** and **Area**. The results added to the Results Table will be available as variables in Equations.

10. Click **OK** to exit the Peak Area/Height dialog.

    The Peak Table tab and Results Table tab are updated.

Area

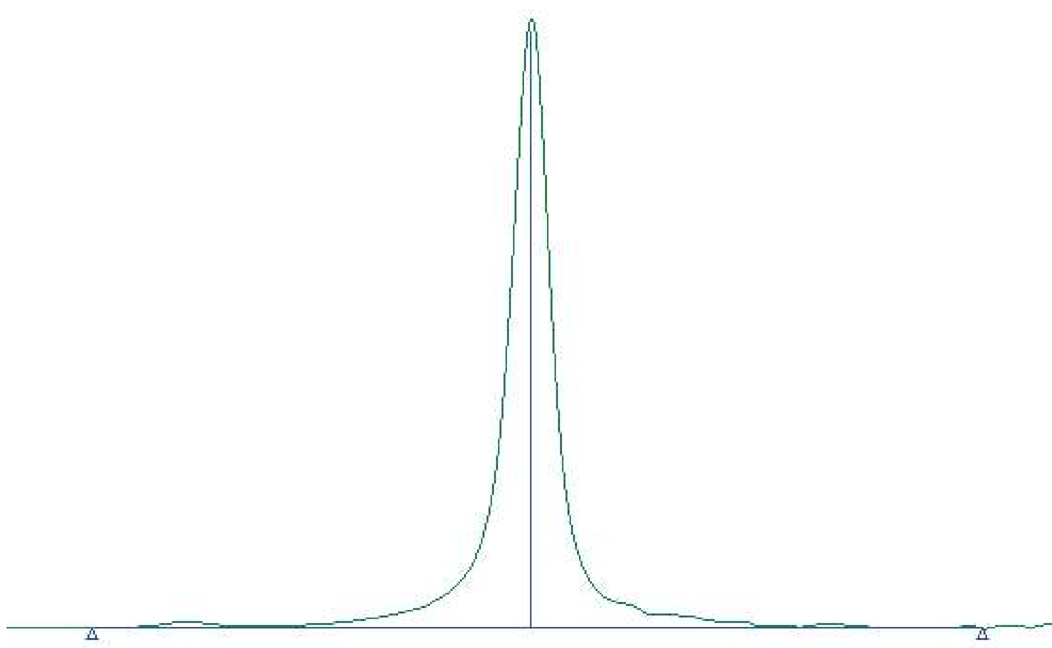
An area is defined by a start and end abscissa value and two base points. Here is an example of the peak area markers:



Height

Height is defined by an abscissa value (X in the table) and two base points. If no bases are selected, the Height is measured from the curve to zero absorbance. If one or two bases are selected, the max height is measured from the curve to the baseline.

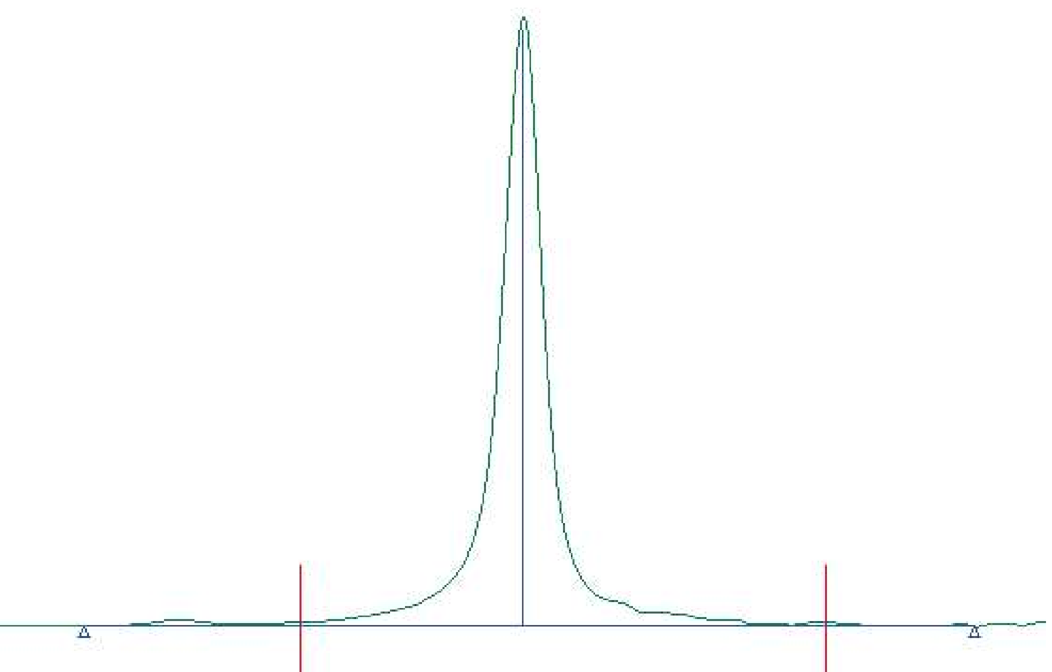
Here is an example of the height markers:



Max height

Max height is defined by a start and end abscissa value and two base points. The **Max Height** is the maximum peak height between the start and end abscissa values. If no bases are selected, the max height is measured from the curve to zero absorbance. If one or two bases are selected, the max height is measured from the curve to the baseline.

Here is an example of the height markers when Max Height is selected:



Defining a Ratio

The Ratio option is only available when two rows are selected in the table.

1. Click in the left-hand column of the peak row that you wish to be the numerator.

   The row is highlighted.

2. Hold down the CTRL button on your keyboard, and then select the left-hand column of the peak row that you wish to be the denominator.

   Both rows are highlighted.

3. Click **Ratio**.

   A new row is added to the table, and automatically named [Peak Name Row 1]/[Peak Name Row 2].

NOTE:	If you modify the parameters of either peak row, then the ratio values are automatically updated.

Removing a Row from the Table

- Select the row or rows in the table containing the peak positions that you want to remove, and then click **Remove**.

Peak Area/Height Results

The results are displayed on the Peak Table tab in the Viewing Area.

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

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

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

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

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

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

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

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

The results are also displayed on the Results Table tab.

Additional Information

The results of the Peak Table process are also added to the Peak Table tab. Each time you run a Peak Table or Peak Area/Height process on a spectrum, a new row is appended to the results for that Samples View.

Quant

Once you have set up Quant, use the Quant process to run the selected Quant method for your samples.

1. Ensure that the **Include** checkbox for each Quant method that you want to run is enabled on the Setup Quant Methods tab, and that parameters such as Pathlength are entered correctly.
2. Select **Quant** and then **Quant Analysis** from the Process menu.

   OR

   Click the icon on the Process bar.

   The Quant process is performed, and the results are displayed on the Quant tab.

Quant Results

The Quant results are displayed on the Quant tab.

- Your Quant results for each Spectrum are tabulated in the upper left quadrant of the Quant tab.

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

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

  To view this table in detail, it may be helpful to drag the borders between the quadrants.
- The Details for each result are tabulated in the upper right quadrant of the Quant tab. These include the Pathlength and any Bias Correction settings.

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

  To view this table in detail, it may be helpful to drag the borders between the quadrants.
- The sample spectrum and, if generated, the Residual spectrum and Calculated spectrum for the Quant result selected are displayed in a graph below the Quant Results.

  The Residual spectrum is named r_[Sample Name].sp and the Calculated spectrum is named c_[Sample Name].sp.

  You can drag the Residual and Calculated spectra from the graph window onto the Samples View.

  The **Show Calculated Spectra** and **Show Residual Spectra** checkboxes enable you choose whether to display these spectra.

See Setup Report Defaults for details of how to select which results are displayed by default and which made available in the column selector.

The Quant results are also available in the Equation Variables list on the Setup Equation Properties dialog and in the Results Table.

Rejecting a Quant Result

- Right-click the result that you want to reject in the Quant results table (in the upper left quadrant of the Search tab), and then click **Delete result** in the shortcut menu.

NOTE:	If you have Spectrum ES software, you cannot delete results.

Rejecting all Quant Results

To complete the Quant Process by rejecting all the results:

- Right-click any result in the Quant results table (in the upper left quadrant of the Search tab), and then click **Delete all results** in the shortcut menu.

NOTE:	If you have Spectrum ES software, you cannot delete results.

Additional Information

The Quant results for each algorithm are displayed in the following table:

Algorithm	**Results generated per method**	**Results generated per Component/Property**
Beer's Law		% Value, Prediction Error
PLS1	RMS error, P2P (Peak-to-peak) error, Total M-distance, Residual ratio	%Value, Prediction Error, M-distance, residual spectrum and calculated spectrum.
PLS2	RMS error, P2P (Peak-to-peak) error, Total M-distance, Residual Ratio	%Value, Prediction Error, M-distance, residual spectrum and calculated spectrum.
PCR+	RMS error, P2P (Peak-to-peak) error, Total M-distance, Residual Ratio	%Value, Prediction Error, M-distance, residual spectrum and calculated spectrum.
QuantC	RMS error, P2P (Peak-to-peak) error, F value, % Variance	%Value, Prediction Error

RMS error

The RMS (Root Mean Square) residual is a measure of the average error (standard deviation) associated with the residual spectrum. This value should be comparable to the RMS noise level in the unknown spectrum.

Peak-to-Peak error

The P2P (Peak-to-Peak) error represents the maximum range of deviation between the original (unknown) spectrum and the calculated spectrum (maximum residual – minimum residual). Typically, this value should be in the order of five times the RMS error if the residuals consist of only random noise. A high value for the P2P error can indicate that there are features in the unknown sample that were not present in the calibration set. It is advisable to view the residual spectrum to determine the origin of the unmodeled feature.

Total M-distance

The Total M-distance ratio is the ratio between the Mahalanobis distance for the unknown sample and the leverage cutoff. The leverage cutoff reflects twice the average leverage of the calibration standards. A value significantly greater than 1 for the Total M-distance ratio may indicate that the unknown sample lies outside the calibration set. In such cases the prediction results must be treated with caution. The Total M-distance ratio may exceed 1 if there are additional overlapping features in the unknown spectrum that have not been modeled, or if the modeled features are more intense than those in the calibration set (extrapolation). The residual ratio enables you to distinguish between these two cases. Additional unmodeled features in the unknown spectrum which do not overlap will not affect the M-distance, but will increase the residual ratio.

Residual Ratio

The Residual Ratio is the ratio of the residual variance of the unknown to the residual variance of the calibration standards. A high value compared to those seen for independent validation standards suggests that the residual spectrum contains features not modeled during calibration. In such cases, the prediction results should be treated with caution and the features in the residual spectrum investigated.

% Variance

The % Variance summarizes the amount of spectral variance of the unknown described by the standards. If the unknown is one of the standards, this is 100%.

F-value

The F-value summarizes the model-to-noise spectral variance as described by analysis of variance (ANOVA). High F-values correspond to the unknown sample being well-modeled by the standards.

See the Quant Builder on-screen Help file for mathematical definitions of these terms.

Compare

Once you have set up compare references, use the Compare process to:

- Compare one spectrum with another.
- Compare one spectrum with a directory of spectra.

The Compare process estimates the similarity between two spectra. One or more filters emphasize the features in the spectra that relate to the chemical composition of the sample, and reduce the contribution of features that have other causes.

1. Display and select the spectrum or spectra that you want to process.
2. Select **Compare** from the Process menu.

   OR

   Click on the Process bar.

The results are displayed on the Compare tab in the Viewing Area.

- While the comparisons are being processed a progress bar is displayed at the bottom of the Compare tab, together with a **Cancel** button.
- Your results and the referenced spectra are tabulated at the top of the Compare tab. To view these tables in detail, you can drag the bottom border of the tabulated area, or the border between the tables.
- Your source spectrum and any referenced spectra are displayed in a graph below the results tables.
- You may stop the process at any time; the results already obtained are displayed.
- Use the shortcut menu to select to send the Compared References spectra to the Samples View.
- You can drag-and-drop spectra from the graph to the Samples View.

Rejecting a Compare Result

➢ Right-click the result that you want to reject in the Source Spectra Compare Results table (in the upper left quadrant of the Compare tab), and then click **Delete Selected Result** in the shortcut menu.

NOTE:	If you have Spectrum ES software, you cannot delete results.

Rejecting all Compare Results

To complete the Compare Process by rejecting all the results:

➢ Right-click any result in the Source Spectra Compare Results table (in the upper left quadrant of the Search tab), and then click **Delete All Results** in the shortcut menu.

NOTE:	If you have Spectrum ES software, you cannot delete results.

Additional Information

Correlation

A correlation of 1.0 indicates that there is a perfect match between two spectra as the two data sets are identical. In practice this is extremely unlikely, and probably means that the two spectra are copies of the same spectrum.

A correlation of zero indicates that the two spectra are wholly unrelated. This is also unlikely because there are almost always some small similarities between spectra.

The Compare Process

The Compare process uses absorbance spectra so that differences in concentration or pathlength are overcome. The correlation coefficient is calculated by the following expression:

$$\text{Correlation} = \frac{\sum w_i A_i B_i}{(\sum w_i A_i A_i)^{1/2} \times (\sum w_i B_i B_i)^{1/2}}$$

where A_i and B_i are the absorbance values in spectra A and B at frequency i, and w_i is a weighting that depends on the filters selected.

When more than one filter is used, the total weighting is the product of the weightings of the individual filters.

Search

Once you have set up spectral libraries and search parameters, use the Search process to perform a Euclidian search of the included Search Libraries.

Search for Spectra

To perform a Euclidian search of the included Search Libraries:

1. Display and select the Samples View, or one or more spectra within a Samples View, that you want to search for.
2. Select **Search** from the Process menu.

   OR

   Click on the Process bar.

   The Search process is performed, and the results displayed on the Search tab in the Viewing Area.

While your search is being processed a progress bar is displayed at the bottom of the Search tab, together with a **Cancel** button. You can cancel the process at any time; the results already obtained are displayed.

Search Results

The Search results are displayed on the Search tab.

- Your Source Spectra Search Results (that is, the best hits for each spectrum in turn) are tabulated in the upper left quadrant of the Search tab.

  To view this table in detail, it may be helpful to drag the borders between the quadrants.
- The Search Hit List spectra are tabulated in the upper right quadrant of the Search tab.

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

  Use the shortcut menu to send the Search Hit List spectra to the Samples View.
- The best hit spectra are displayed in a graph below the Source Spectra Search Results, in the lower left quadrant of the Search tab.

  You can drag-and-drop spectra from the graph to the Samples View.
- Any Additional Property information that is included with the Search Result, such as a physical property, is tabulated below the Search Library References, in the lower right quadrant of the Search tab.

Accepting an Alternative Search Result

By default the highest scoring best hit is recorded in a set of columns in the Results Table tab. If you decide that the highest scoring best hit for a sample is inappropriate, you can accept another hit:

1. Select the **Search** tab, and then make sure the appropriate row is selected in the Source Spectra Search Results table (in the upper left quadrant of the Search tab).

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

2. Select your preferred row from the Search Hit List table (in the upper right quadrant of the Search tab), and then click **Accept as best hit**.

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

Rejecting a Search Result

- Right-click the result that you want to reject in the Source Spectra Search Results table (in the upper left quadrant of the Search tab), and then click **Delete Selected Result** in the shortcut menu.

NOTE:	If you have Spectrum ES software, you cannot delete results.

Rejecting all Search Results

To complete the Search Process by rejecting all the results:

- Right-click any result in the Source Spectra Search Results table (in the upper left quadrant of the Search tab), and then click **Delete All Results** in the shortcut menu.

NOTE:	If you have Spectrum ES software, you cannot delete results.

Search Residuals

If the components of a mixture do not interact significantly with each other, they can be considered as a linear combination of components. By performing successive search and difference process steps, you are able to sequentially remove the major components of your mixture and then search for the minor components from what is left (the residuals). As Search is a correlation-based process, it will preferentially suggest the major components of a mixture. Thus, removing these increases the chance of correctly identifying the minor components. This semi-automated components analysis gives you full control over which components are subtracted, and the weighting of that difference process.

Search Residuals enables you to find the Best Hit for your spectrum, then use the Difference process to subtract that Best Hit spectrum from your sample spectrum. You can then perform another search on the difference spectrum:

1. Select the **Search** tab, and then make sure the appropriate Sample is selected in the Source Spectra Search Results table (in the upper left quadrant of the Search tab).
2. Select your preferred row from the Search Hit List table (in the upper right quadrant of the Search tab), and then click **Mixture Search**.

   The Difference dialog is displayed in the Viewing Area. This dialog contains interactive controls below a **Split** view; the upper graph display contains the two source spectra, and the lower graph contains the calculated difference spectrum.
3. Enter any scaling **Factor** you want applied to the **Spectrum to subtract.**

   OR

   Click **Auto.**

   The scaling factor is calculated automatically by performing a least squares fit of the two source spectra.
4. Click **Search Again** to perform a search on the Difference result.

   The Difference dialog is closed, the Search process is performed against the difference spectrum (that is, the processed Source spectrum), and the results are displayed on the Search tab in the Viewing Area. The difference spectrum is added to the Samples View.
5. Repeat Steps 2-4, as required.

Shortcut Menus

On the Search tab, the list of Source Spectra Search Results (top left quadrant), Search Library References (top right quadrant), and Additional Property (bottom right quadrant) includes a shortcut menu that enables you to copy one or more table rows to, for example, Excel.

The graph of best hit spectra includes a selection of tools and a shortcut menu that enable you to optimize and label the graph, and copy it to the Windows clipboard to be pasted into, for example, Word. You can also use the shortcut menu to send the Search Hit List spectra to the Samples View.

- To access a shortcut menu, right-click in the appropriate quadrant.

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

Additional Information

Spectral Libraries

If you want to browse the contents of, or edit, a spectral library, select it from the Spectral Libraries area of the Navigation pane.

MultiSearch

NOTE: You can only run MultiSearch if you have entered a valid license number for this feature during the installation of your software.

MultiSearch enables you to identify up to ten components in a mixture, and estimate their percentage levels. Once you have selected the search libraries and decided if any spectra should be included or excluded by default, you can run the MultiSearch process and then view the results spectra.

1. Display and select the Samples View, or one or more spectra within a Samples View, that you want to analyze using MultiSearch.

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

   OR

   Click on the Process bar.
   The MultiSearch process is performed, and the results displayed on the MultiSearch tab in the Viewing Area.

While your search is being processed, a progress bar is displayed at the bottom of the MultiSearch tab, together with a **Cancel** button. You can cancel the process at any time; the results already obtained are displayed.

MultiSearch Results

The MultiSearch results are displayed on the MultiSearch tab.

- The MultiSearch Results (that is, the best hits for each spectrum in turn) are tabulated in the upper left quadrant of the MultiSearch tab.

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

  You can select which columns to display in the table using the column selector in its top left corner. The **MultiSearch Score** is a value for the overall match between the result and the sample, analogous to the Score from the Search process. The **Level** is the estimated concentration of each component in the mixture, in %. The **MultiSearch Cumulative Score** shows how the step-by-step addition of each component to the mixture affects the fit to the sample spectrum.

- The MultiSearch Hit List spectra are tabulated in the upper right quadrant of the MultiSearch tab.

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

  You can also choose to view hits containing a specified number of components from the **Components in hit** drop-down list.

  Right-click an entry and select **Send to Samples View** to send the MultiSearch Hit List spectra to the Samples View.

- The results spectra are displayed in three tabs below the MultiSearch Results, in the bottom half of the MultiSearch tab.

  Fitted displays the sample spectrum and the fitted spectrum of the mixture components identified in the hit.

Components displays a split view of the sample spectrum and the identified mixture components spectra, each scaled according to their calculated level.

Residuals displays a series of residual spectra for the fitting of each identified component spectrum in turn to the sample spectrum.

NOTE: If one or more spectra were included in the search by default, the names of these spectra are marked with an asterisk (*) in the results tables.

Accepting an Alternative Search Result

By default the highest scoring best hit is recorded in a set of columns in the Results Table tab. If you decide that the highest scoring best hit for a sample is inappropriate, you can accept another hit:

1. Select the **MultiSearch** tab, and then make sure the appropriate row is selected in the MultiSearch Results table (in the upper left quadrant of the Search tab). When a Samples View is selected, the MultiSearch Results table in the MultiSearch tab refers to every sample in the Samples View. If you select a sample from the Samples View, the MultiSearch tab refers to the selected sample.

2. Select your preferred row from the MultiSearch Hit List table (in the upper right quadrant of the MultiSearch tab), and then click **Accept as best hit**.
   The corresponding search result cells in the Results Table tab are updated to refer to the accepted hit.

Further Data Processing

After reviewing your results, you can choose to run MultiSearch again while excluding one of the spectra identified in the original results for that hit, if you suspect that this material may have been incorrectly identified.

1. Right-click the hit in the MultiSearch Hit List table, and select **Exclude Spectrum.**
   A list of the components of the hit is displayed.
2. Click the spectrum you want to exclude.
   The MultiSearch process automatically repeats with this spectrum excluded.

NOTE: Changes made to the excluded spectra in the MultiSearch tab do not affect the Setup MultiSearch tab settings.

Verify

Verify allows methods developed using PerkinElmer's AssureID software to be run using Spectrum. Once you have set up the Verify method, use the Verify process to determine whether your sample matches any of the materials in the method (identification), or whether it is an acceptable example of a specified material (authentication).

NOTE: You can only run one Verify method at a time.

1. Select **Verify** from the Process menu.

   OR

   Click in the Process toolbar.

   OR

   Right-click on the sample spectrum in the Samples View tab and select **Verify**.

   A sub-menu appears showing the Verify methods from the table in the Setup Verify tab.

   NOTE: Verify is only available as a Process option when at least one method has been added to the Setup Verify tab.

2. Click the method you want to run.

   If the method contains only one material, the Verify process runs and the results are displayed on the Verify tab.

3. If the method contains more than one material, select the material you want to use from the second sub-menu that appears (for authentication).

   OR

   Select **Unspecified** (for identification).

Running Verify in a macro

If you are using a macro to run a Verify method that contains more than one material, you might have to select the material from a list in the sample table each time the macro is run, depending on how the macro is set up. This will be indicated by a message that there are errors in the sample table. If you attempt to scan without selecting the target material, a message is displayed that there are errors in the sample table.

1. Click **Sample Table** in the Data Explorer pane.
2. Click the Specified Material column cell for the Verify method in the sample table (it will be highlighted in red), and select one of the options from the drop-down list.
3. Click **Scan** in the Measurement toolbar to continue running the macro.

Verify Results

The results from the Verify process are displayed on the Verify tab.

- The Verify results for each spectrum are tabulated in the upper left panel of the Verify tab.

  This table lists the **Sample Name**, the Verify **Method Name**, the **Material Type Specified** in the method, and the result of the method under **Identified As**. If a specific material was selected for authentication, the table also shows whether the sample has passed (been authenticated as the selected material) or failed.

- The Details for each result are tabulated in the upper right panel of the Verify tab. These include the numerical results associated with the method, which will depend on the type of algorithm used (see Additional Information below).

- The sample spectrum is displayed in a graph below the Verify results.

  The **Show Mean Spectrum** checkbox enables you to choose whether or not to display the mean spectrum for the specified or identified material with the sample spectrum.

Additional Information

The numerical results reported in the Details pane of the Verify tab depend on the algorithm used by the method.

For the COMPARE algorithm, the correlation and correlation threshold are displayed.

- Correlation is a measure of the similarity of the material mean spectrum and the sample spectrum, regardless of the relative sizes of the peaks.

- Correlation threshold is the limit below which the material mean spectrum and sample spectrum are judged to be different.

For the SIMCA algorithm, the total distance ratio, distance ratio limit, model distance and residual distance are displayed.

- The total distance ratio, model distance and residual distance measure the difference between the material model and the sample.

  The lower these numbers, the closer the sample is to the material.

- The distance ratio limit defines the threshold above which the sample spectrum is judged to be outside the material's variation and, therefore, does not belong to that material.

Adulterant Screen

NOTE: You can only run Adulterant Screen if you have entered a valid license number for this feature during the installation of your software.

Adulterant Screen examines a sample spectrum for the presence of specific adulterants that you have selected as being of particular concern for your sample. Once you have set up the Adulterant Screen method for a particular sample material, you can screen a sample of the material to determine if it contains any of the selected adulterants, and estimate the levels present as a proportion of the corresponding adulterant spectrum.

NOTE: You can only run an Adulterant Screen for one material at a time.

1. Select **Adulterant Screen** from the Process menu.

   OR

   Click in the Process toolbar.

   OR

   Right-click on the sample spectrum in the Samples View tab and select **Adulterant Screen**.

   A sub-menu displays the materials available in the Setup Adulterant Screen tab.
2. Select the material corresponding to your sample to run Adulterant Screen.

Adulterant Screen Results

The key results that are generated by Adulterant Screen are:

- Level

  This is the amount of adulterant(s) present in the sample expressed as a proportion of the adulterant spectrum used in the screening process. If the adulterant spectrum is of a pure substance and is collected under the same conditions as the sample, then this value will be approximately equal to the concentration of adulterant in the sample. Differences in the purity of the adulterant, pathlength, sampling accessory, etc., will cause deviations from this value. In particular, the effective pathlength in diffuse reflectance measurements depends on the scattering properties of the sample, so the level will correspond only approximately to the concentration when using this technique.
- Confidence

  This is a measure of the reliability of the adulterant detection. It is affected by the calibration of the material model, and whether the adulterants have spectral features that are sufficiently distinctive from the material and (for multiple adulterants) each other. It is an experimentally-derived measure that is not simply related to any standard statistical definition of confidence.

The results from the Adulterant Screen process are displayed on the Adulterant Screen tab.

- By default, the table lists the **Sample Name**, the filename(s) of the **Adulterant** identified, the adulterant **Level**, **Confidence**, **Material Fit**, **Adulterant Screen Pass/Fail** and **Unidentified Components.** The Adulterant Screen Pass/Fail column displays whether the sample is a **Pass** or **Fail**, depending on whether it has identified that any of the selected adulterants exceed the fail limits in the setup (if these are enabled). If fail limits are not enabled then the table displays **No Limits Selected.** The Material Fit column describes how closely the sample spectrum fits the model of the sample material (**Normal**, **Marginal** or **Abnormal**). If none of the selected adulterants have been detected but the Material Fit is Marginal or Abnormal, then it is possible that the sample contains other impurities. The likelihood of this is indicated by the rating in the Unidentified Components column (**Unlikely**, **Possible** or **Probable**). You can choose to add other columns using the column chooser in the top left corner of the table. Refer to Troubleshooting results for more details.

- The Details for each result are tabulated in the upper right panel of the Adulterant Screen tab.

  For each sample, the table lists the hits that comply with the Results Display settings in the setup. The adulterant(s) identified is reported, with the corresponding level and confidence. You can also choose to display the residual and the detection limit for each hit using the column chooser in the top left corner of the table. The residual indicates how closely the hit matches the sample spectrum; the smaller the residual, the closer the match. The detection limit for each adulterant is calculated by the algorithm based upon the validation of the material model.

  The Details table will automatically list the hits for a particular sample in descending order based on the confidence and the residual from the algorithm. The first item in the list is always the "no adulterants" case; that is, the fit to the material model assuming that no adulterants are present. The Residual is displayed for this item, and if the Material Fit is Abnormal (meaning that the sample spectrum contains features that are not due to the sample material) then this is listed in the Confidence column. The second item in the list (if present) is the best hit. To change the best hit, select a different result and click **Accept Best Hit**. The results in the left panel and the Results Table will be updated automatically.

  You can also sort the data in this table by clicking the column headers. The adulterant names are sorted alphabetically. The levels are sorted numerically by the total values for the adulterant(s) in the sample. The detection limit values are sorted numerically by the first value in each cell. The confidence levels are sorted alphabetically. The residual values are sorted numerically.

  NOTE: If there are errors in the Adulterant Screen process, then these are shown in the processing log.

- A number of different spectra are displayed to provide assistance with interpreting the results of the process. These are shown on three tabs:

  Fitted: The preprocessed sample spectrum is shown. This tab also displays the sample spectrum calculated (fitted) by the Adulterant Screen algorithm both before and after including the adulterants identified by the screening process. If the calculated spectrum including adulterants is a closer match to the sample spectrum than the calculated spectrum excluding adulterants, then this is an indication that the adulterants are present in the sample.

Residual: The residual spectrum before fitting adulterants is displayed, which shows the features from the sample spectrum that are not included in the material model. This tab also displays the same spectrum after the identified adulterants have also been removed (residual spectrum including adulterants). If the residual spectrum including adulterants contains almost no distinct features, then this is an indication that the adulterant is present in the sample. If some spectral features remain, they may indicate that other adulterants or contaminants are present, that the model of the sample material does not account for all the possible sources of variation in the sample, or that the wrong material model has been used.

Adulterants: The combined spectrum of the identified adulterant(s) scaled with respect to the calculated level is displayed. This tab also displays a calculated (fitted) version of this spectrum generated from the sample spectrum by the algorithm. If these two spectra are similar in appearance, then this is another indication that the adulterant is present in the sample.

Refer to Troubleshooting results for more details.

NOTE: If no adulterants are detected above the result display limits set in the Process Parameters tab, then only the first two tabs of spectra are displayed, and neither contains any spectra where adulterants are fitted to the sample.

NOTE: If you select **First derivative** in the Process Parameters tab when setting up the Adulterant Screen material, then only first derivative spectra will be displayed in the results.

Changing the Best Hit

After reviewing the results, you can change the best hit chosen by the software:

1. Click the result you want to choose as the best hit in the Adulterant Screen details panel.
2. Click the **Accept as Best Hit** button.

   The results in the left panel and the Results Table are updated to show the new best hit.

Additional Information

Possible errors

One example of an error in Adulterant Screen occurs when the detection limit of an adulterant is higher than the fail limit. If the measured concentration is in between these two values, then the pass/fail result is unreliable. You should either increase the fail limits in the Adulterant Screen setup, or attempt to reduce the detection limit by using more calibration and validation samples to improve the material model.

Troubleshooting results

It is important to critically review the results obtained from Adulterant Screen to make sure that they are not misinterpreted. The adulterants identified and the Adulterant Screen Result only refer to the adulterants included in the process. You need to use the Material Fit and Unidentified Components results, together with the graphs, to decide if there are any other problems with your sample, as described below:

The Material Fit will be Marginal or Abnormal if there is anything in the sample that is not described by the model of the material. There are three possible sources of such a discrepancy:

1. One or more of the adulterants in the screening process are present in the sample at higher than trace levels.
2. Other adulterants or contaminants that are not included in the setup are present in the sample.
3. The sample material does not match the material in the calibration samples.

The first cause should be revealed by the adulterants identified. The second and third causes will be indicated if the Unidentified Components column displays **Possible** or **Probable**. The residual including the adulterants will also be high.

If the Unidentified Components column displays a **Possible** rating, then it may be because there are other adulterants present that are similar to those selected for the screening process. It may also indicate that the adulterant spectrum is being affected by interactions with the sample (for example, hydrogen bonding with aqueous liquids), or that the crystalline form of the adulterant is different. Finally, where there are multiple adulterants present in the sample, one of them may not have been included in the list of adulterant spectra.

Where the rating is **Probable**, this may indicate that another substance is present that is quite dissimilar to the other adulterants, or that the wrong material has been used either in the setup or the sample. It is not usually possible to distinguish between additional adulterants or an incorrect material using Adulterant Screen. A Verify method could be set up to check that the sample falls within the normal variation for your product before running an Adulterant Screen. If appropriate, improve the material model in Adulterant Screen by using more calibration and validation samples which cover all sources of variation in the material, or exclude the spectra of any obvious outliers.

Equations

Equations are process commands that perform calculations on one or more spectra, or on the data obtained from other processes. An equation must be defined before it can be used.

To apply an equation that you have previously defined:

1. Display and select the spectrum or result that you want to process.
2. Select **Equations** from the Process menu, and then click on the name of the equation that you want to apply.

   OR

   Select the =√λ icon labeled with the name of the equation that you want to apply from the Equations drop-down list on the Process bar.

   By default, an Equation icon and label is added to the Equations drop-down list on the Process bar each time a new equation is defined.

   The Results Table tab is updated. If the result amends the source spectrum, the processed spectrum is displayed in the Viewing Area and added to the Samples View.

Processed spectra are not saved to disk automatically.

Additional Information

Defining Equations

For further information about adding a new equation, see Setup Equations.

For further information about modifying an equation, see Setting up an Equation.

For further information about formatting the numeric results obtained by applying an equation, see Formatting Equation Results.

Macros

Macros are process commands that apply a previously defined series of other process commands.

To apply a Macro that you have previously defined:

1. Display and select the spectrum or spectra that you want to process.
2. Select the **Macros** sub-menu from the Process menu, and then click on name of the Macro that you want to apply.

   OR

   Click the icon on the Process bar and then click on the name of the Macro that you want to apply.

   By default, a Macro icon and label is added to the Macros sub-menu of the Process bar each time a new Macro is defined.

   As each process in the Macro is completed, the Results Table tab is updated, and the processed spectrum is added to the Samples View and displayed in the Viewing Area. This enables you to examine the intermediate results in the Macro, as well its final results.

   Processed spectra are not saved to disk automatically.

Additional Information

Data Collection with Macros

If your macro includes a Data Collection step, the Data Collection is controlled using the buttons on the Measurement bar. If **Show prompt at start of step** was selected in the setup, a message will be displayed informing you that a Data Collection step is in progress. If **Show sample table** was selected in the setup, the Sample Table tab will be displayed. If not, the Live tab will be displayed during the scan. Follow the instructions on the Prompts Display to collect your spectra.

Click on the icon to access the options **Run next step**, which enables you to go to the next step, or **Stop macro**.

Select **Run next step** to exit the Data Collection and to proceed with any subsequent macro steps.

NOTE: If **Mandate all samples** was selected in the setup, then **Run next step** is not available. When all the spectra in the Sample Table have been collected the macro will continue to the next step automatically.

Macros Results

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

  This enables you to examine all the intermediate spectra and results.
- For spectra, or results, generated during a Macro step to be added to the Samples View and displayed in the Viewing pane, or the Results table, **Visible** should be enabled in the Macro Settings dialog. If Visible is not selected, the result of the step will still be available for the next step of the Macro.
- If you apply a Macro to more than one spectrum, the Macro is applied step-by-step to each spectrum.
- If you include a Search process in your Macros, its results are displayed in the Search tab.
- If the Results table becomes overly complex, consider hiding (or resizing) the columns containing intermediate results.

Defining Macros

For further information about entering, or modifying a Macro, see Setting Up Macros.

Biodiesel Macros

If you have the Biodiesel Analyzer installed, two Macros are listed in the Process menu and are available as icons on the Process Bar. The two Macros, Biodiesel HATR and Biodiesel UATR are for FAME (ASTM D7371) analysis for data collected using HATR and UATR, respectively.

Quant Method Wizard

Quant Method Wizard

The Quant Method Wizard enables you to create a new Quant method directly from your spectra, without needing to open the Spectrum Quant software application. You need to build a method using a set of standard spectra that have different known values of each property of interest.

After defining the standards that will be used, set up the parameters for the prediction, including the baseline and the region(s) of the spectra you are going to use.

Open spectra in Spectrum Software and ensure that they are selected.

1. Select **Quant** from the Process menu, and then select **Quant Method Wizard** from the sub-menu.

   OR

   Click the icon on the Process bar, and then select **Quant Method Wizard** from the drop-down.

   The Welcome to Spectrum Quant Method Wizard page is displayed.

2. Select **Create New Method**.
3. Click **Next**.

   The **Algorithm Type** page is displayed.

4. Select an **Algorithm Type** from the drop-down list.

   Beer's Law algorithm is available by default. If you have acquired the Quant Algorithm Pack, then the following algorithms will also be available: PCR+, PLS1 and QuantC.

5. Click **Next**.

   The Standards page is displayed, which contains a list of the spectra you selected.

   A property column, Property1, is already added to the table, which you can rename. If your spectra contained any custom columns, these are also added to the table.

6. If you did not select any spectra before running the Wizard, or you would like to add any additional spectra, click **Add Standards**.

   The Add standard spectra dialog is displayed.

7. Browse to and select the spectrum or spectra you would like to add, and then click **Open**.

   The spectra added are listed in the Standards table.

   If the Assign sample custom fields to properties dialog is displayed, refer to Adding Standards with Custom Fields.

8. Click **Add Column** to add any additional columns you require to define the properties for the prediction.

   As well as adding further property columns, you can also add a Normalization column You can normalize your standards by multiplying the each property value by a scaling factor, for example, the pathlength for the measurement.

9. Enter the property values for your standards.
10. Enter any normalization factor for your standards.
11. Ensure that **Edit Method Parameters** is selected.
12. Click **Next**.

The Algorithm Parameters page is displayed showing the appropriate algorithm parameters.

For the Beer's Law algorithm, a tab is created for each property defined on the Standards page.

13. Set up the algorithm parameters.

    Refer to Beer's Law Parameters for details of the peak and regression parameters for the Beer's Law algorithm.

    Refer to the Spectrum Quant on-screen help for details of the parameters for the PCR+, PLS1 and QuantC algorithms.

14. If you are using the Beer's Law algorithm, repeat Step 13 for each property.

15. Click **Next**.

    The Pre-Processing page is displayed.

16. Select the options to be used on the Summary tab, and then configure the parameters on the tabs for each option.

    The options available will depend upon the selected algorithm. Refer to the Spectrum Quant on-screen help for details of the parameters available for each algorithm, and how to configure them.

17. Click **Next**.

    The Calibration page is displayed.

18. Click **Calibrate** to run the calibration.

    The results of the calibration are displayed in the Calibration Summary. This provides details of the method, algorithm parameters, pre-processing options, calibration results, and the specified and estimated (calculated) property values and residuals for each standard.

19. To view the results of each property, select the appropriate option from the **Select Property** drop-down list.

20. Click **Next**.

    The Save page is displayed.

21. Enter a **Method Name**.

    Any additional information can be entered in the **Method Description** field.

22. Select a save **Location** from the drop-down list.

Browse	Opens the Browse for Folder dialog. Navigate to and open the folder where you want to save the method.
Private	The Private folder location is specific to the user: For Windows 7/8: C:\ProgramData\PerkinElmer\Quant\Users\<User name>\methods For Windows XP: C:\Documents and Settings\All Users\Application Data\PerkinElmer\Quant\Users\<User name>\methods
Public	The Public folder is visible to all users and was specified during installation of Spectrum software. The default location is C:\pel_data\Quant\Methods

23. Click **Finish** to save the method and exit the Quant Method Wizard.

    If you have Spectrum Quant ES, you may be prompted to enter an electronic signature for the Save Method signature point.

    The method will be saved in the *.qmd format.

Standards

The Standards table enables you to select the spectra to be used as calibration standards in your model.

NOTE: A column selector in the top left corner of the Standards table enables you to define which columns are displayed by selecting the appropriate check box. The options are: Exclude, Name, Data/Time, File Path, and any property columns.

Adding, Removing and Excluding Standards

Adding Standards

1. Click **Add Standards.**
   The Add standard spectra dialog is displayed.
2. Select the spectra to be used as standards and then click **Open.**

   By default, binary spectra (*.sp files) are displayed. You can also open interferograms (*. ig files), JCAMP-DX files (*.dx, *.jdx), Omnic files (*.spa), GRAMS (*.spc), or spectra saved as data points in a PerkinElmer ASCII text format (*.asc files).

   If you have Spectrum Quant ES, you may be prompted to enter an electronic signature for the Open non-ES Data signature point.

   A row is added to the Standards table for each spectrum selected.

NOTE: If the Assign sample custom fields to properties dialog is displayed, refer to Adding Standards with Custom Fields.

Adding Standards with Custom Fields

If your spectra have Custom Fields associated with them, you can set up a Property or Normalization column for the Custom Field. You can create a new column, or select an existing column. If you do not want to include data in a Custom Field, you can select to Ignore it.

1. Click **Add Standards.**

   The Add standard spectra dialog is displayed.
2. Select the spectra to be used as standards and then click **Open.**

   The Assign sample custom fields to properties dialog is displayed, which lists the Custom Fields for the selected spectra.
3. For each Custom Field select the **Type** of column you want to create in the table.

   The options are **Property** or **Normalization.** If you do not want to add a column for the Custom Field to the Standards table, then select **Ignore.**

4. If you want to create a new column in the Standards table, with the column name set to the name of the Custom Field, then ensure that **Use existing column** is not selected.

   OR

   To use an existing column, select the **Use existing column** check box and then select the appropriate **Property Name** from the drop-down list.

   If Normalization was selected as the column Type, and there is already a Normalization column in the table, then **Use existing column** will be selected. The **Property Name** option will be blank.

5. Click **Accept.**

   The spectra are added to the Standards table, and the data in the Custom Field for the spectra selected are added either to a new column with the same name, or to the column with the Property Name selected.

   OR

   To ignore data in all Custom Fields, click **Ignore.**

   The spectra are added to the Standards table, but any data in Custom Fields will be ignored.

Selecting Rows

- Select, or deselect, a complete row in the table by clicking the first (left most) column in the row.

  Any selected rows (or cells) are highlighted.

- To select a block of rows, hold down the SHIFT key and click the first column in the first row and last rows, or click and drag up or down the table.
- To select a row, or deselect a row leaving the others selected, hold down the CTRL key as you click the rows.

Selecting Columns

- Select, or deselect, a complete column in the table by clicking the column header.

  Any selected cells are highlighted.

Removing Standards

1. Select the standards that you want to remove.

2. Click **Remove Standards.**

   The Remove Standards dialog is displayed.

3. Click **Yes.**

   The selected standards are removed from the Standards table.

Excluding Standards

To exclude one or more standards from the calibration:

- Select the appropriate **Exclude** check box next to the standard you want to exclude.

  The standard will not be included in the calibration. It is not removed from the Standards table.

Adding a Property Column

NOTE: A property column (**Property1**) is added to the Standards table by default. You can rename a property.

1. Click **Add Column**.
2. Select **Add Property** from the drop-down list.

   The Add Property dialog is displayed.
3. Type the **Property Name** and **Units**.
4. Click **OK** to add the Property Name as a column in the Standards table.

   The units are displayed in parentheses after the Property Name in the column header.

   To enter, or edit, the value of any property, double-click the left mouse button in the appropriate cell and then type the required value.

Adding, Renaming and Deleting A Property using the Context menu

To Add a property:

1. Right-click on the column header of an existing property column and select **Add Property**.

   The Add Property dialog is displayed.
2. Type the **Property Name** and **Units**.
3. Click **OK** to add the Property Name as a column in the Standards table.

   The units are displayed in parentheses after the Property Name in the column header.

   To enter, or edit, the value of any property, double-click the left mouse button in the appropriate cell and then type the required value.

To Rename a property:

1. Right-click on the column header of the property column and then select **Rename Property**.

   The Rename Property dialog is displayed.
2. Type the new **Property Name** and, if required, type the new **Units.**

3. Click **OK** to apply the changes to the column in the Standards table.

   OR

   Click **Cancel** to exit the dialog without saving the changes.

To Delete a property:

1. Right-click on the column header of the property column and select **Delete Property**.

   The Remove Column dialog is displayed.

2. Click **Yes** to remove the column from the Standards table.

   OR

   Click **No** to exit the dialog without saving the changes.

Adding a Normalization Column

You can normalize your standards by multiplying the each property value by a scaling factor. The default scaling factor is 1.

The main reason for using a scaling factor is when you wish to use pathlength normalization. In this case, type the pathlength for each standard in the Normalization column.

1. Click **Add Column**.

2. Select **Add Normalization** from the drop-down list.

NOTE: There can be only one Normalization column in the Standards table. If a Normalization column has already been added to the table, then the Add Normalization option will not be available.

   The Normalization column is added to the Standards table. The default value is 1.

3. To change the Normalization value, select the cell and type a new value.

Removing Columns

1. Select the column that you want to remove by clicking on the column header.

2. With the column selected, click **Remove Column**.

   The Remove Column dialog is displayed.

3. Click **Yes** to remove the column from the Standards table.

   OR

   Click **No** to exit the dialog without saving the changes.

Beer's Law Parameters

If Beer's Law is selected as the Algorithm, you need to set up the peak and regression parameters for each property defined in the Standards table.

Selecting a Spectrum

Before defining the peak parameters, select an appropriate Standard spectrum to display:

- Select the spectrum you want to view from the **Select spectrum for parameter display** drop-down list.

Setting the Peak Parameters

You can calculate the property values using a peak area or a peak height (either the height at a defined abscissa value or the maximum height over a range). The values can be measured from zero absorbance or from a user-defined baseline. You can also calculate the property using the average of two peaks, using the Peak Ratio option.

You can use the Vertical Cursor and the markers on the graph to define the peak parameters. Alternatively, you can just type the values you want directly into the table. The graph display will be updated accordingly.

To define the Peak Parameters:

1. Select **Area**, **Height** or **Max Height** as the Peak Type.

   Area calculates the area under the curve over a selected range. Height determines the height of the selected peak. Max Height determines the maximum peak height over a selected range.

2. If you want to calculate a peak ratio, select **Peak Ratio**.

   A row is added to the peak table for the second peak and a row is added for the ratio. The ratio is automatically named [Peak Name Row 1]/[Peak Name Row 2].

   You can edit the name of a peak. Click the left mouse button in the appropriate cell and type a new name.

3. Select the number of Bases for the **Baseline**.

   If no bases are selected, the zero absorbance is used as the baseline.

   If Base 1 only is selected, then a horizontal baseline is drawn at the ordinate value defined on the graph. If Base 1 and Base 2 are selected, the baseline is drawn between the two points defined on the graph.

   If one or more bases are selected, then the options **Min Bases** and **Mean Bases** become available.

   Min Bases adds range markers for each base point (displayed on the graph as two hollow triangles). The base point used (marked on the graph by a solid triangle) is the minimum value between the markers.

   Mean Bases adds range markers for each base point (). The base point used (not marked on the graph) is the mean value between the markers.

4. If you selected Peak Ratio in Step 2, select the row in the table for the first peak you want to define.

5. Move the Vertical Cursor to the peak position you want to use to calculate the property, and then double-click to add the peak position to the table.

Position the mouse pointer over the Vertical Cursor until the mouse cursor changes to a double-headed arrow ⇔. Hold down the left mouse button and then move the mouse left or right to drag the cursor to the new position. Release the mouse button. Then double-click the left mouse button. The values in the peak table are automatically updated.

NOTE: The peak position must be in the range of all the spectra included in the Standards table.

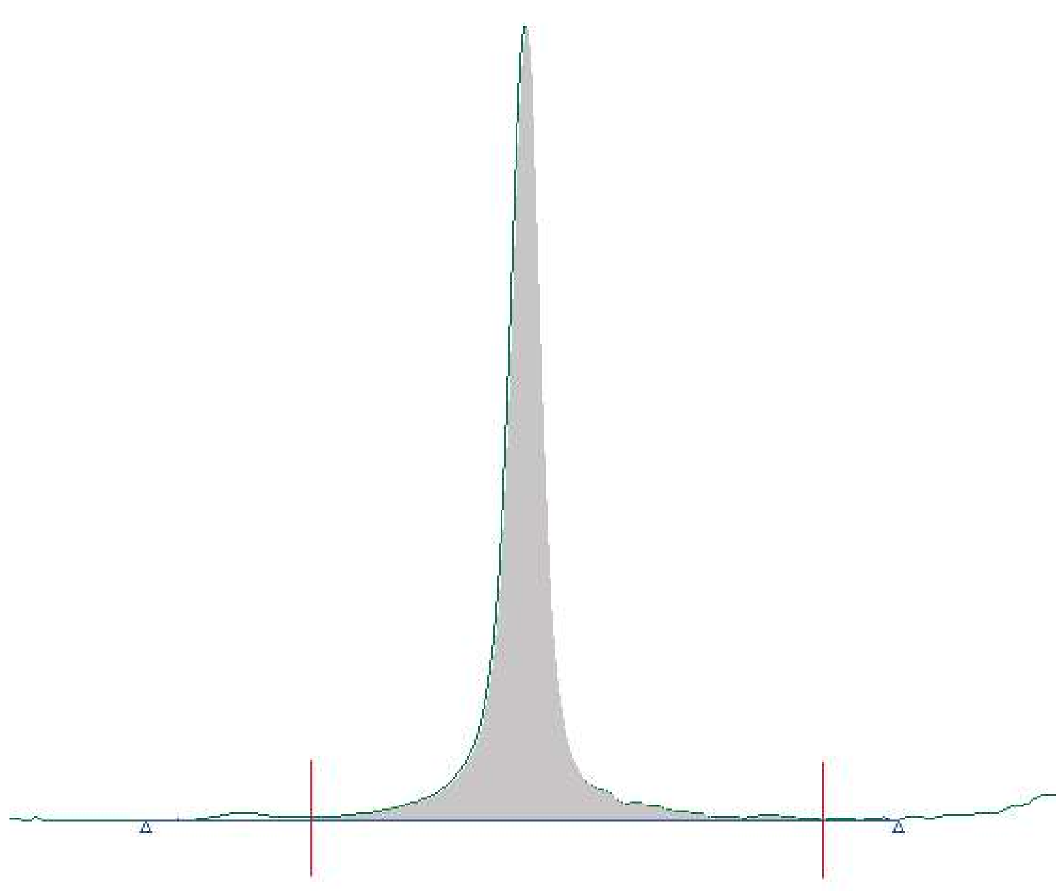
6. Use the graph markers to adjust the point on the curve at which the height will be determined, the range over which the peak area or maximum height will be calculated, or the position of the baseline markers, as required.

To move a range or baseline marker, hover the cursor over it until a double-headed arrow ⇔ is displayed, click the left mouse button and then drag the marker to the new position on the curve. Release the left mouse button. The values in the peak table are automatically updated. Alternatively, you can just type the values you want directly into the table. The graph display will be updated accordingly.

Area

Area is defined by Start and End abscissa values (displayed as vertical lines on the graph). If no bases are selected, then the Area is measured from the curve to zero absorbance. If one or two bases are selected (shown as triangles on the graph), then the Area is measured from the curve to the baseline.

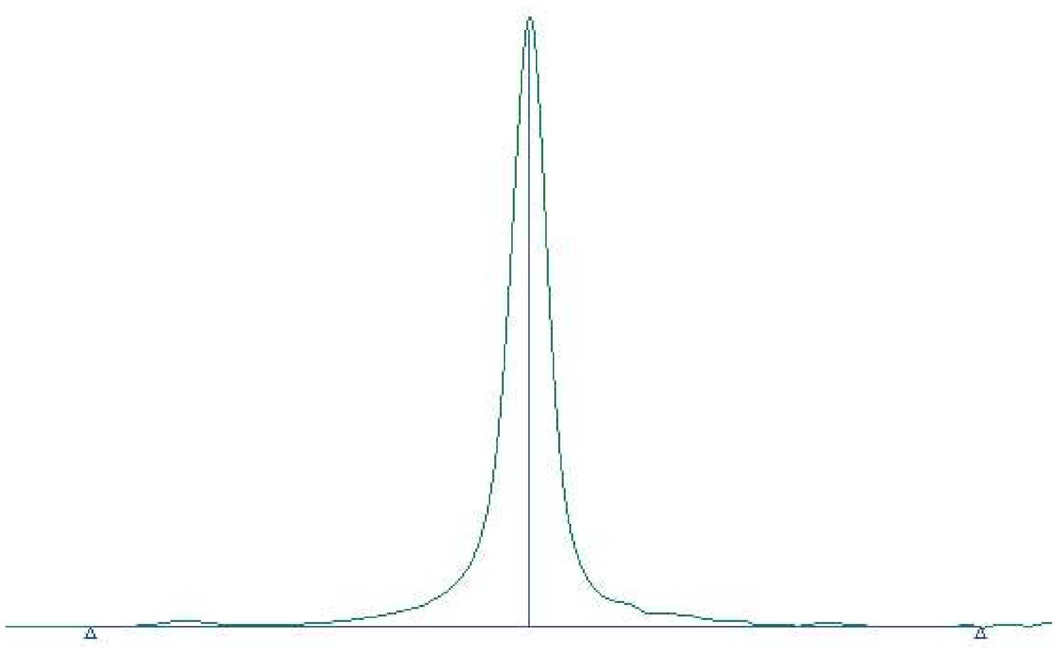
Here is an example of the peak Area markers with two base points.



Height

Height is defined by an abscissa value (X in the table). If no bases are selected, then the Height is measured from the curve to zero absorbance. If one or two bases are selected (shown as triangles on the graph), then the Height is measured from the curve to the baseline.

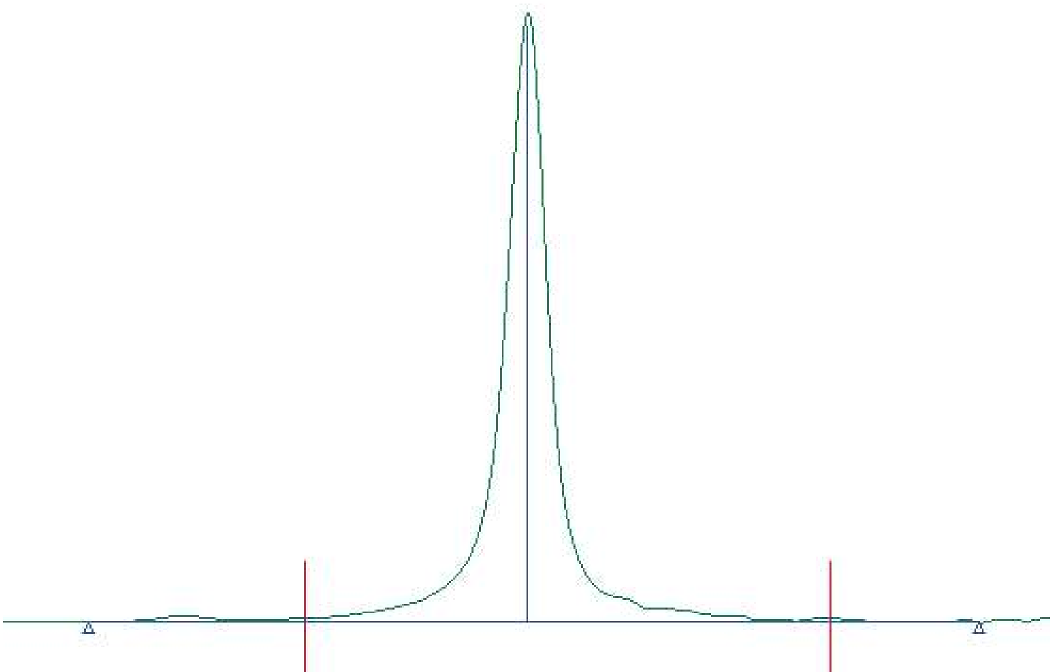
Here is an example of the Height marker with two base points.



Max Height

Max Height is defined by Start and End abscissa values (displayed as vertical lines on the graph). The Max Height is the maximum peak height between the Start and End abscissa values. If no bases are selected, then the Max Height is measured from the curve to zero absorbance. If one or two bases are selected (shown as triangles on the graph), then the Max Height is measured from the curve to the baseline.

Here is an example of the Max Height markers with two base points.



7. If you selected Peak Ratio in Step 2, repeat Steps 5-6 for the second peak.

NOTE: If you modify the parameters of either peak row, then the ratio values are automatically updated.

Setting the Regression Parameters

The Regression Parameters enable you to select the type of fit that will be used in the calibration:

1. Display the **Fit Type** drop-down list and then select the required option.

   The options are **Linear**, **Quadratic**, **Cubic** and **User Defined**.

2. For Linear, Quadratic and Cubic fits, select **Force through zero** if you want to force the fit through the origin.

   OR

   For the User Defined fit, enter appropriate values for the a0, a1, a2 and a3 coefficients.