

Signal to Noise

It is useful to know the ratio of the peak heights to the level of noise in a mass chromatogram, MassLynx provides the Signal to Noise process to do this. Signal to Noise can be accessed from Chromatogram by choosing **Signal to Noise** from the **Process** menu.

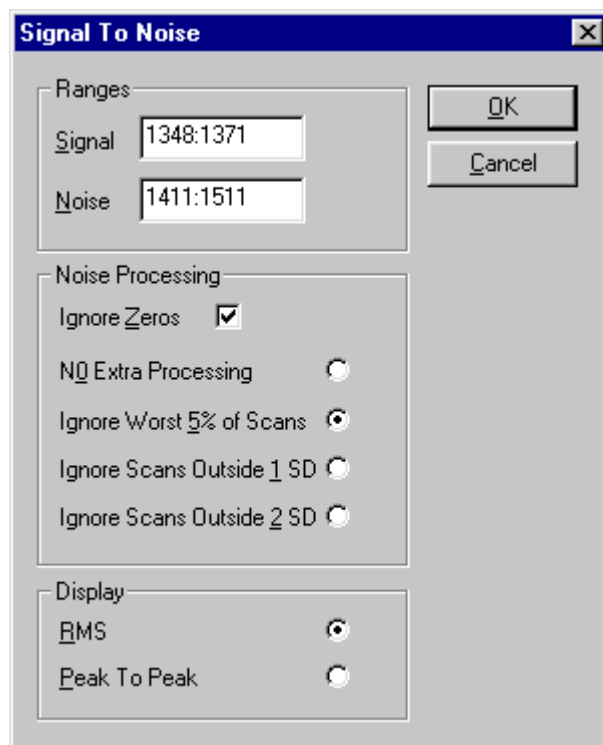


Figure 3.35 Signal to Noise dialog

The Signal to Noise calculations can be carried out to display peak to peak or RMS values. If Peak to Peak is required, the greatest height of the signal range above the mean noise value is divided by the variance. If RMS is required the greatest height of the signal above the mean noise is divided by the root mean square deviation from the mean of the noise. The RMS is usually expected to be 5 times the Peak to Peak value.

Various authorities have different methods for determining what level of noise is taken into account for the calculations of noise variance and RMS deviation. A two step process is carried out. Firstly the mean should be calculated with or without zeros as normal. Optional processing then allows three options:

Ignore Worst 5% of scans The 5% of scans that have the greatest deviation from the mean are disregarded in the noise signal.

Ignore Scans Outside 1SD Those scans whose deviation from the mean is greater than one standard deviation are disregarded in the noise signal.

Ignore Scans Outside 2SD Those scans whose deviation from the mean is greater than two standard deviation are disregarded in the noise signal.

Options 1 and 3 are expected to give roughly equivalent results. Option 2 should give an RMS value of about double that of the other two options.

If one of these three processing options is selected then the mean and RMS deviation of the noise are recalculated disregarding the appropriate points.

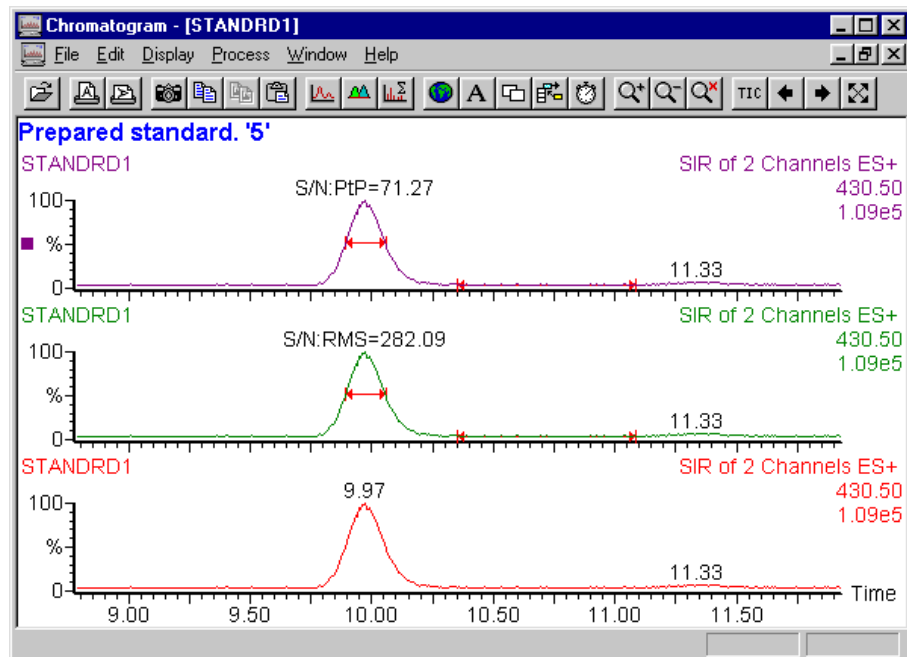



Figure 3.36 Signal to Noise processed chromatogram

- **To calculate the signal to noise value for a mass Chromatogram**
 1. Display the chromatogram range of interest in a chromatogram window.
 2. Choose **Signal to Noise** from the Chromatogram Process menu.
 3. Enter **Signal** and **Noise** ranges. Either type values in or using the mouse press the right mouse button at one end of the Chromatogram region of interest, and without releasing the button, drag the mouse horizontally to the other end. As you drag the mouse you will see a "rubber band" stretched out to indicate the range you have selected. The dialog will be updated to show this range.
 4. Select the **Noise Processing** and **Display** method required.
 5. Press the **OK** button.

Combine Spectra

The **Combine** process can be accessed from either Chromatogram or Spectrum by pressing the  toolbar button or by choosing **Combine** from the **Process** menu.

The combine process operates on centroid-mode or continuum data. Its purpose is to produce a single scan from all the scans across a TIC peak. The combined scan exhibits enhanced signal-to-noise and improved mass accuracy.

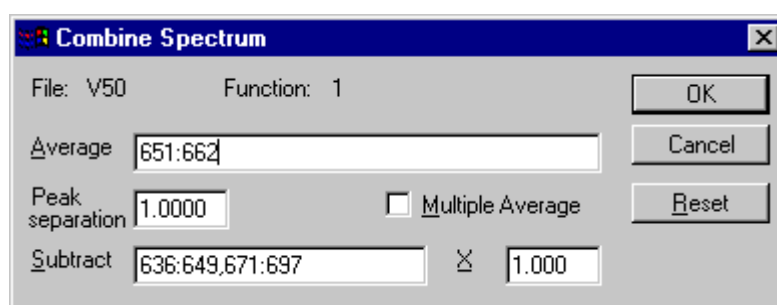



Figure 3.37 Combine Spectrum dialog

You specify three **scan ranges** and a **background factor**. One range contains the scans across the peak top and the other two ranges contain scans from the background, on each side of the peak. The scans across the peak top are averaged together and the average of all the background scans, multiplied by the **background factor (X)**, is subtracted from the result.

Peak separation Enter the parameter of the spectral peak width in amu. For centroided data the peak width can be determined from inspection of the tune peaks in the tune page. The Combine algorithm combines peaks within a **Peak separation** window into a single peak. The **Reset** button will remove all values that have been entered into the dialog.

Normally when using the right mouse button to enter values the first set of values are entered into the Average box and the second and third are entered into the Subtract box. Checking the **Multiple Average** box changes this so that the first six sets of values are entered into the Average box and the seventh and eighth are entered into the Subtract box.

■ To combine scans in a centroid-mode data file

1. Display the chromatogram peak of interest in a chromatogram window.
2. Press the  Toolbar button or choose **Combine spectra** from the **Chromatogram Process** menu.
3. Enter the **peak top scan range** either by typing scan numbers separated by a colon (e.g. 619:626) into the **Average** control, or by dragging across the peak with the right mouse button.
4. Optionally, enter one or two **background scan ranges**. Again, you may do this either by typing scan numbers into the **Subtract** control, or by dragging with the right mouse button. If you type the numbers, each range should be in the form of two numbers separated by a colon, as above, and if there are two ranges, they should be separated by a comma (e.g. 606:612,631:637). If you use the mouse, drag with the right mouse button across the first **background scan range**, then optionally repeat for a second range.
5. Optionally, enter a background factor in the **X** control.
6. Optionally, enter a **Peak separation** value. **Note:** This value allows up to 4 decimal places to allow for accurate mass calculations.
7. Press the **OK** button.