

KnowItAll Mass Spectrometry Training

*Vendor Neutral Data Processing
Solution for Spectral Analyses*

WILEY



KnowItAll™

“ProcessIt for Manual Processing of EI GC-MS Data”

James Little

Mass Spec Interpretation Services

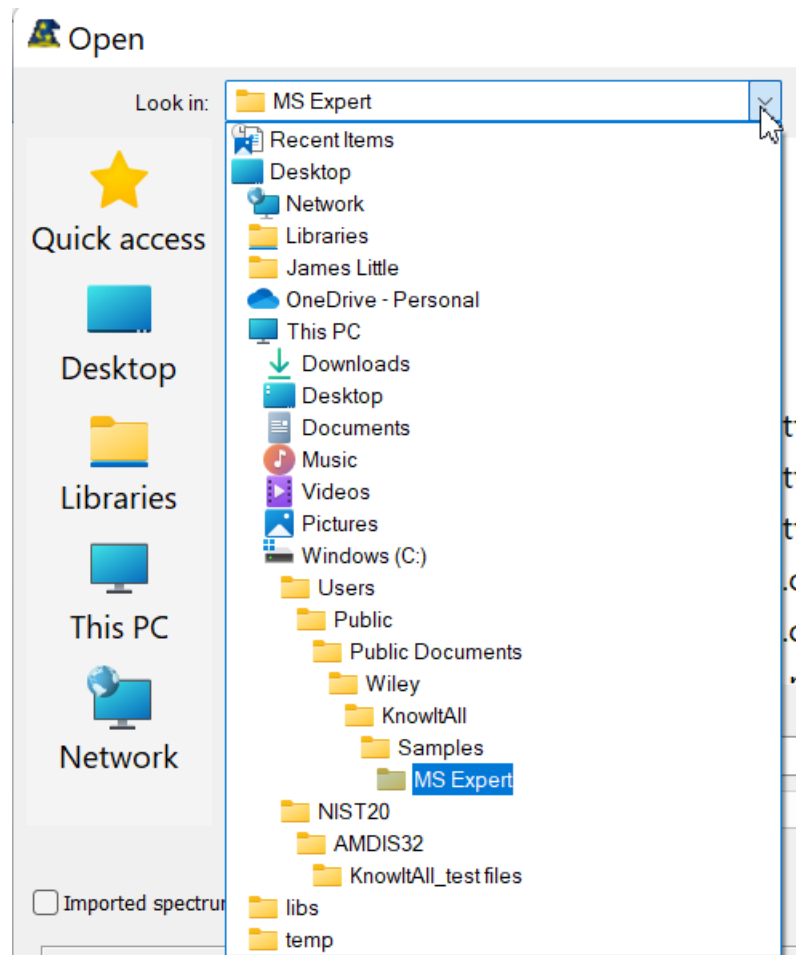
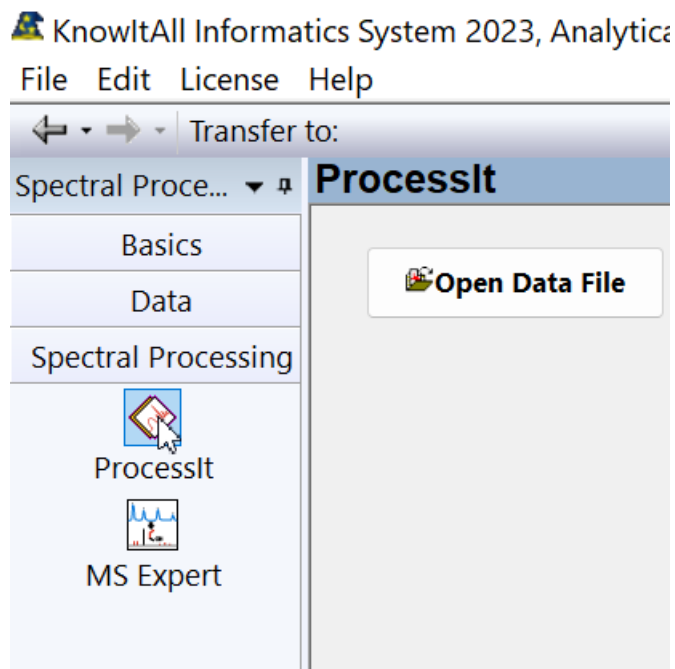
Handouts for Videos:

Website: Little Mass Spec and Sailing

<https://littlemsandsailing.wordpress.com>

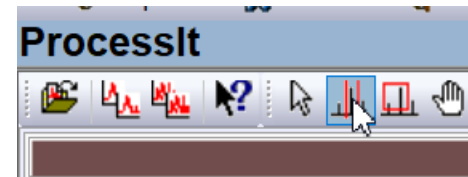
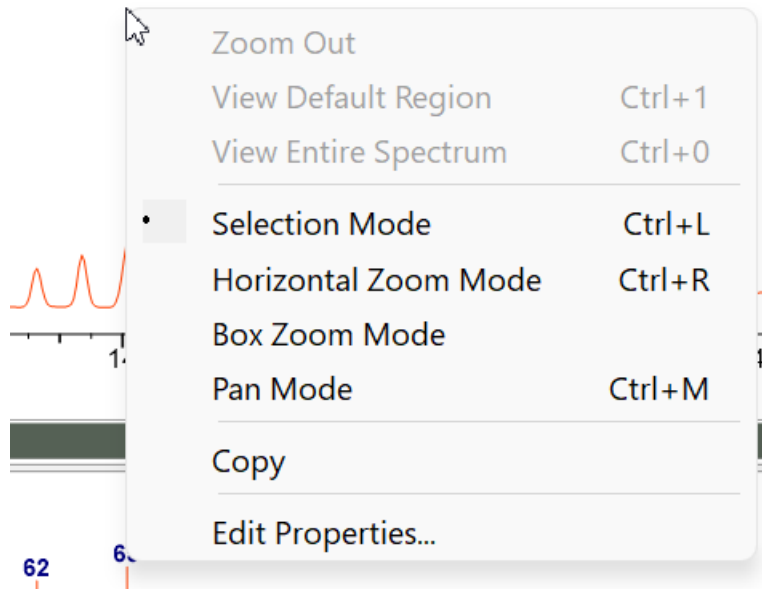
Note: Series of training videos/handouts for KnowItAll mass spectrometry software on my personal web site.

Open ProcessIt In Spectral Processing Group of Programs And Test Files Such as V50.cdf Found in MS Expert Folder

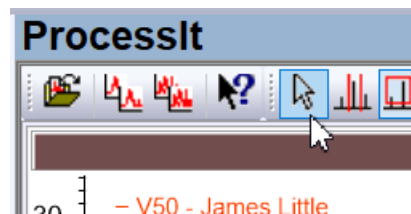
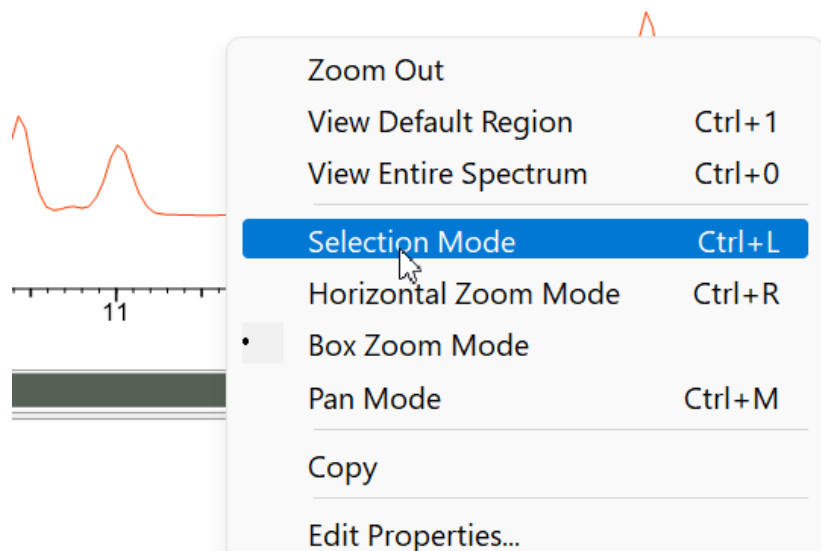


Horizontal Zoom or Box Zoom Mode to Expand Chromatogram

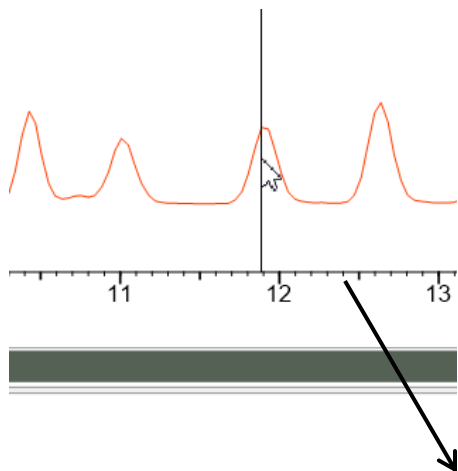
➤ Either right click to select or also found on menu bar



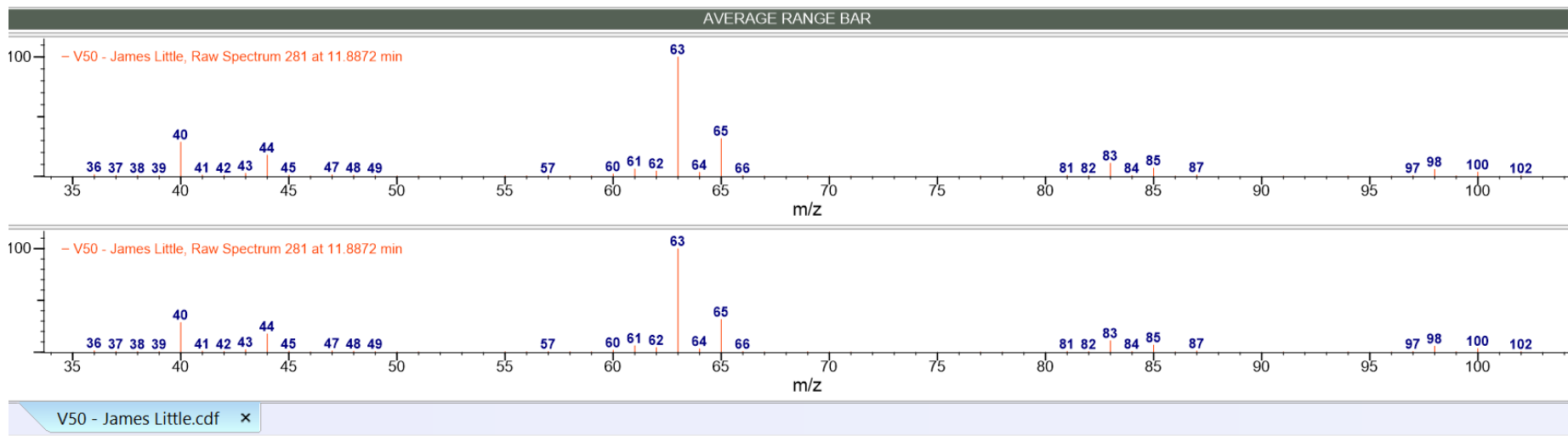
After Zooming, MUST Right Click and Get Select Option to Click on Chromatogram Window to Get a Spectrum or Get Pointer from Menu Bar



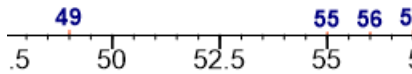
Select Spectrum of Interest by Left Click on Peak of Interest In Chromatogram Window, Sent to Bottom Display



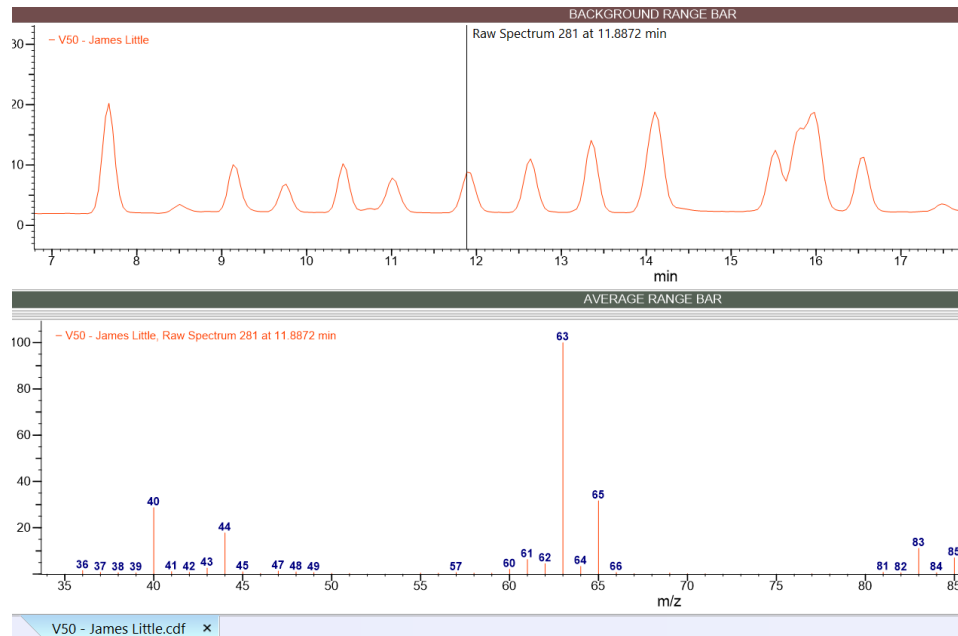
- Selecting peak in this manner does not subtract chemical noise in spectrum
- The top trace in spectrum is the “real time” display noted when the mouse is scrolled over the chromatogram window
- Spectrum is not sent to bottom window until user Left clicks on the chromatogram



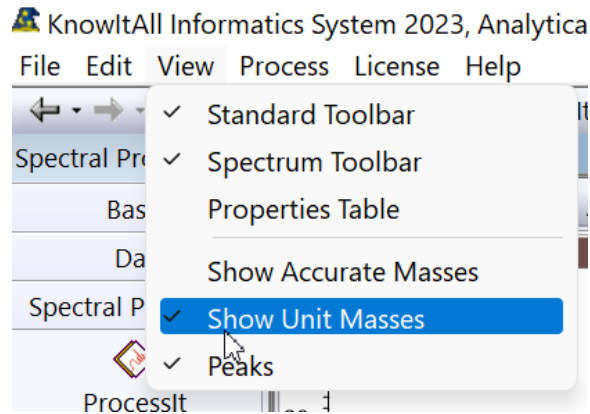
Center Window Can Be Minimized by Hovering Over the Line On the Edge of Its Box to the Mouse Pointer Changes



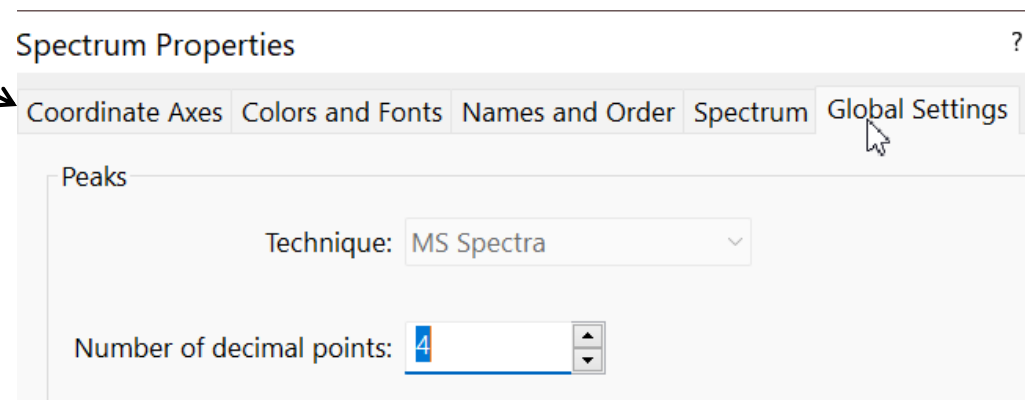
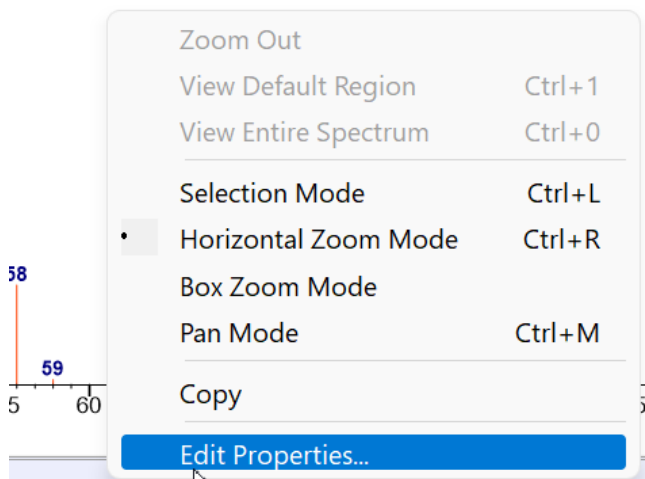
- When mouse button changes, left click and hold to push the window closed
- The spectrum window will only be the one created when left clicking in the chromatogram window
- The dynamic one seen by mouse scrolling will no longer be visible



Select Either Show Unit Masses for Nominal Mass Data or Show Accurate Masses for Accurate Mass Analyses

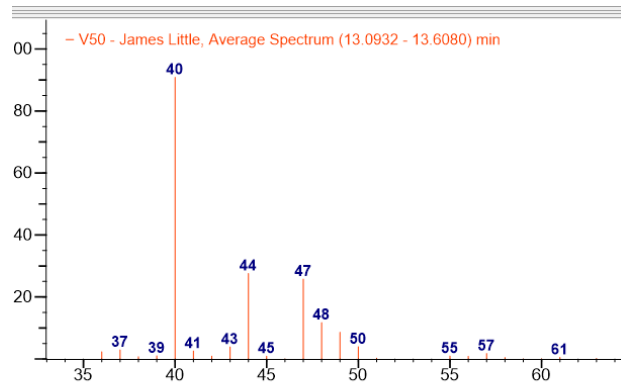
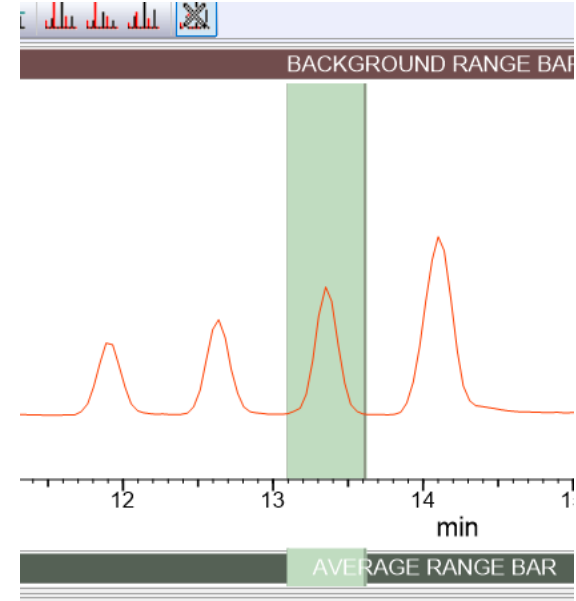
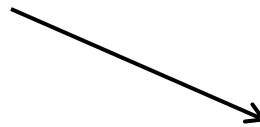
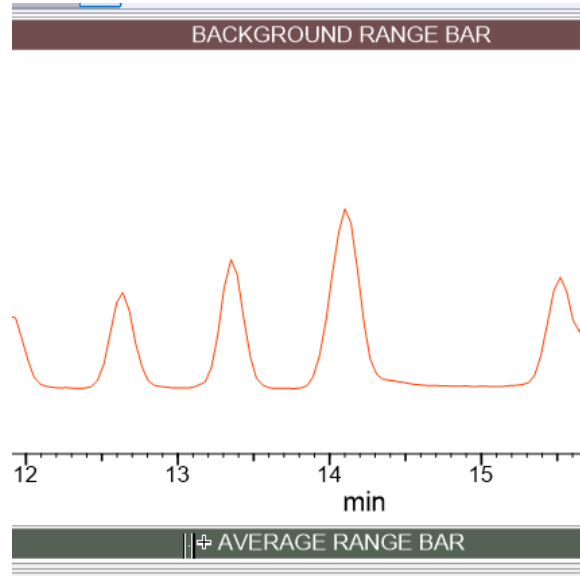


- Select either Unit mass or accurate mass option from View item on menu bar
- Then right click on the spectrum and select Edit Properties
- Then Global tab and usually set number of decimal points as 4
- Can also change other properties for Spectrum
- Can also right click on chromatogram window to change its settings



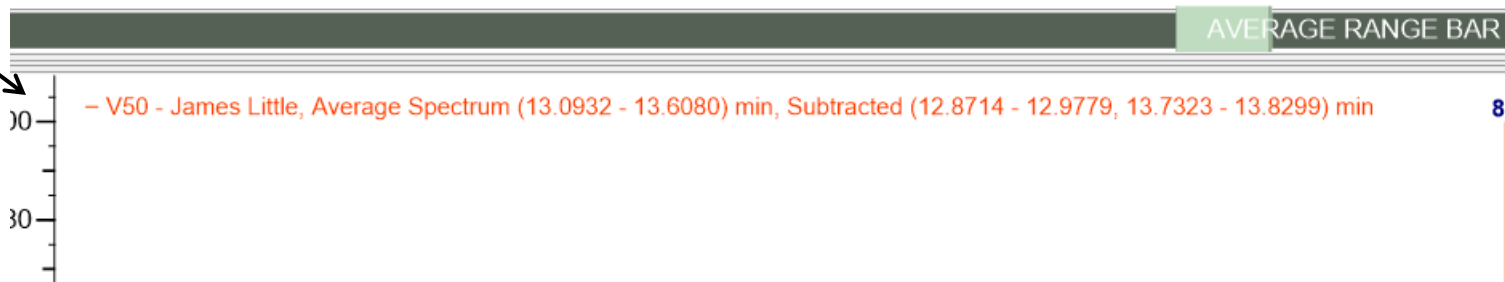
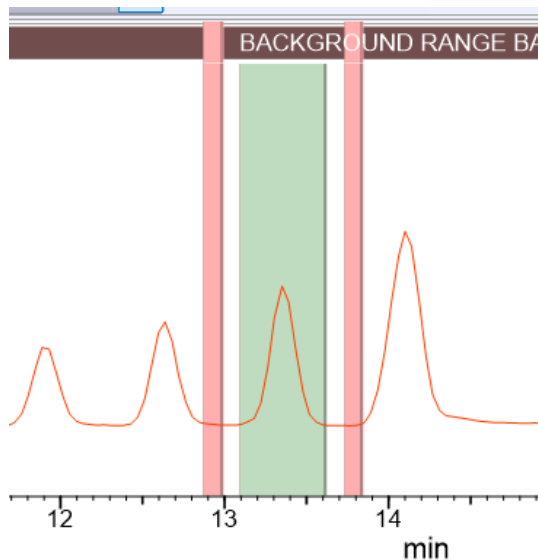
Manually Obtaining Average Spectra Over a Range

- When you hover on the Average Range Bar, one can create one or more averages of combined spectra ranges, one is shown below
- Your pointer MUST be in this bar to accomplish the average spectrum function
- The averaged spectra are sent to the bottom of the window after left clicking and dragging within the bar



Manually Subtracting Background from a Range of Spectra

- After obtaining an averaged range
- Place mouse in the Background Range Bar and left click and drag to determine the background to subtract
- More than one background can be utilized
- The background corrected spectrum is sent to the bottom window

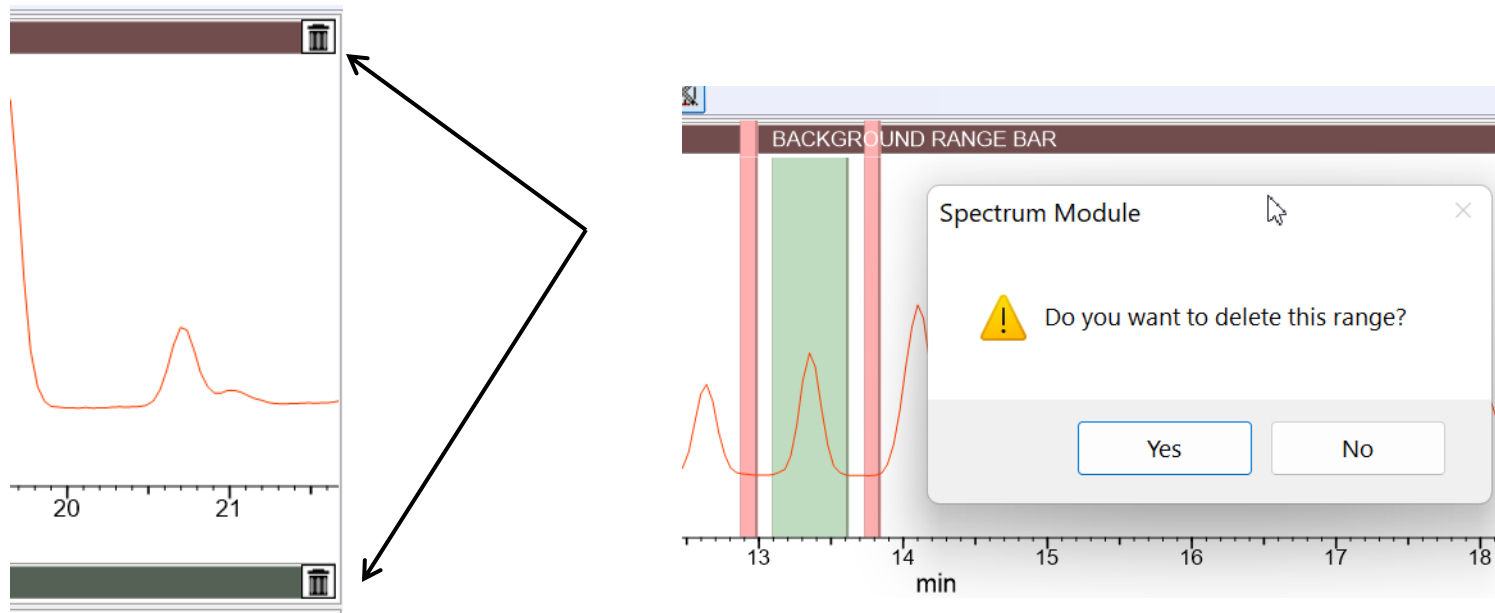


Changing Background and Foreground Ranges

- Can left click on a selected range at the front or rear edge of a box in either the Background Range Bar or Average Range Bar and change its size
- If you left click on center of a range within the either the Background Range Bar or Average Range Bar, you can shift the position of the bar

Removing Background and Foreground Ranges

- Left click in the trash cans at the the Background or Average Range Bar to remove all the ranges
- Or you can right click on either a Background or Average Range in the range bar area and then a box will appear to delete the range of interest



More Than One File Can Be Open at a Time

- More than one file at a time can be open, and you can switch between them from the tabs at the bottom of the window

