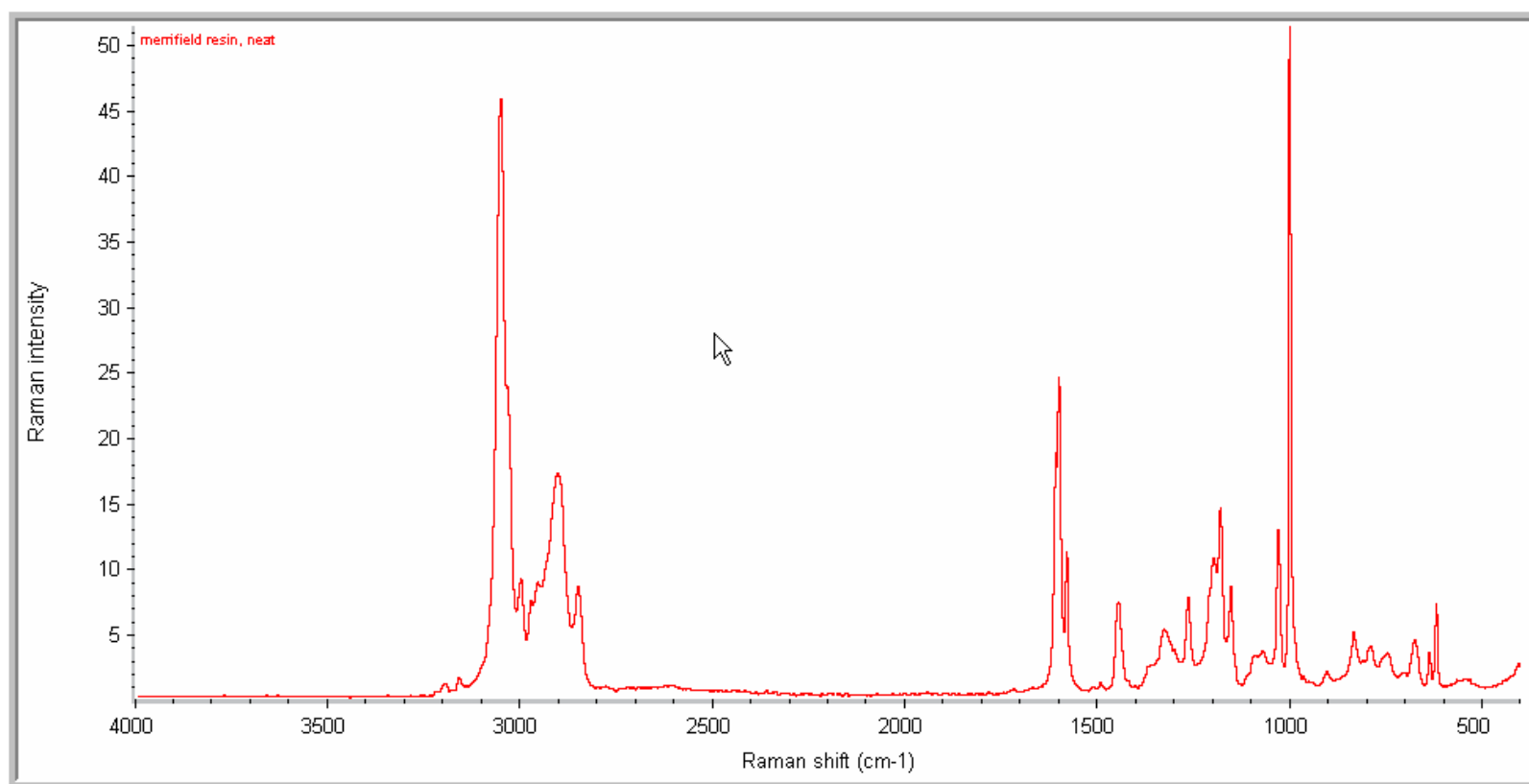


How to Process Raman Data

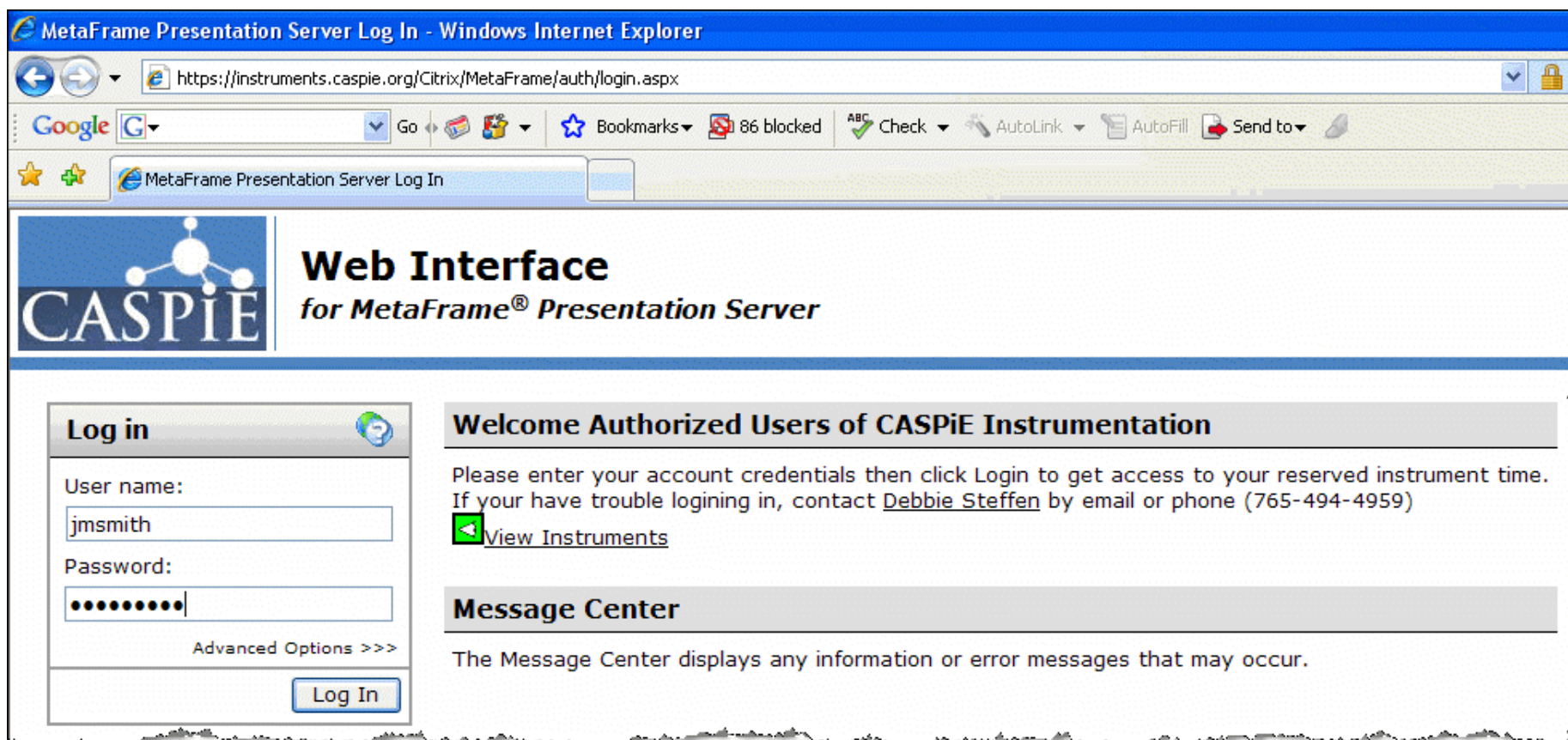
After you run the Raman instrument to collect spectra for your samples you need to mark peak positions and print your data.

You will use a copy of the Raman software that *is not attached to the instrument* to print your spectra.



Load the CASPiE Instrument Site

- To open the Raman data processing software launch your web browser and navigate to the CASPiE instrument website at <https://instruments.caspie.org>.
- Enter your account information to login.



The screenshot shows a Windows Internet Explorer browser window titled "MetaFrame Presentation Server Log In". The address bar displays the URL "https://instruments.caspie.org/Citrix/MetaFrame/auth/login.aspx". The browser's search bar contains "Google" and the address bar includes navigation buttons (Go, Back, Forward), a star icon for bookmarks, and a notification for "86 blocked" items. The main content area features the CASPiE logo on the left and the heading "Web Interface for MetaFrame® Presentation Server". Below the heading is a "Log in" section with a user name field containing "jmsmith", a password field with masked characters, and a "Log In" button. To the right of the login form is a "Welcome Authorized Users of CASPiE Instrumentation" section with a message and a "View Instruments" link. Below that is a "Message Center" section with a brief description.

MetaFrame Presentation Server Log In - Windows Internet Explorer

https://instruments.caspie.org/Citrix/MetaFrame/auth/login.aspx

Google G

Go

Bookmarks

86 blocked


Check

AutoLink

AutoFill

Send to

MetaFrame Presentation Server Log In

 **Web Interface**
for MetaFrame® Presentation Server

Log in

User name:
jmsmith


Password:
●●●●●●●●

Advanced Options >>>

Log In

Welcome Authorized Users of CASPiE Instrumentation

Please enter your account credentials then click Login to get access to your reserved instrument time. If you have trouble logging in, contact [Debbie Steffen](#) by email or phone (765-494-4959)

 [View Instruments](#)

Message Center

The Message Center displays any information or error messages that may occur.

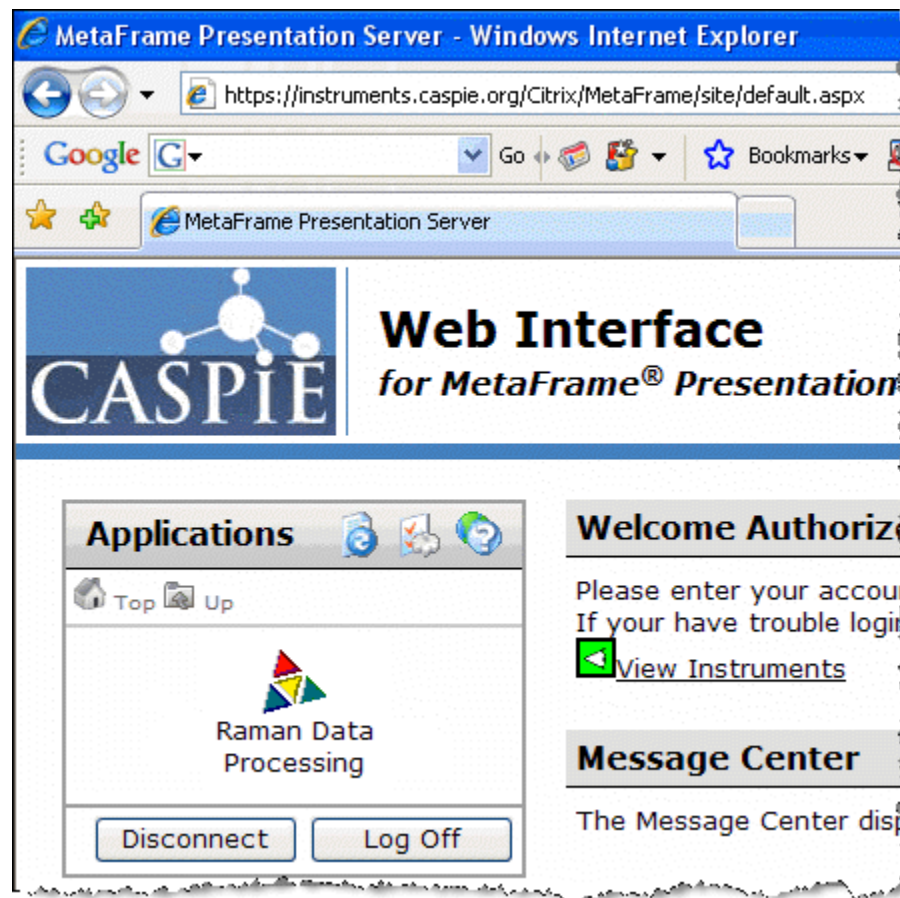
The Raman Data Processing Software



The version of the software not attached to an instrument is called 'Raman Data Processing'.

You will always have access to the Raman data processing software during a CASPIE module. You will only have access to the Raman instrument for remote control during your scheduled hours.

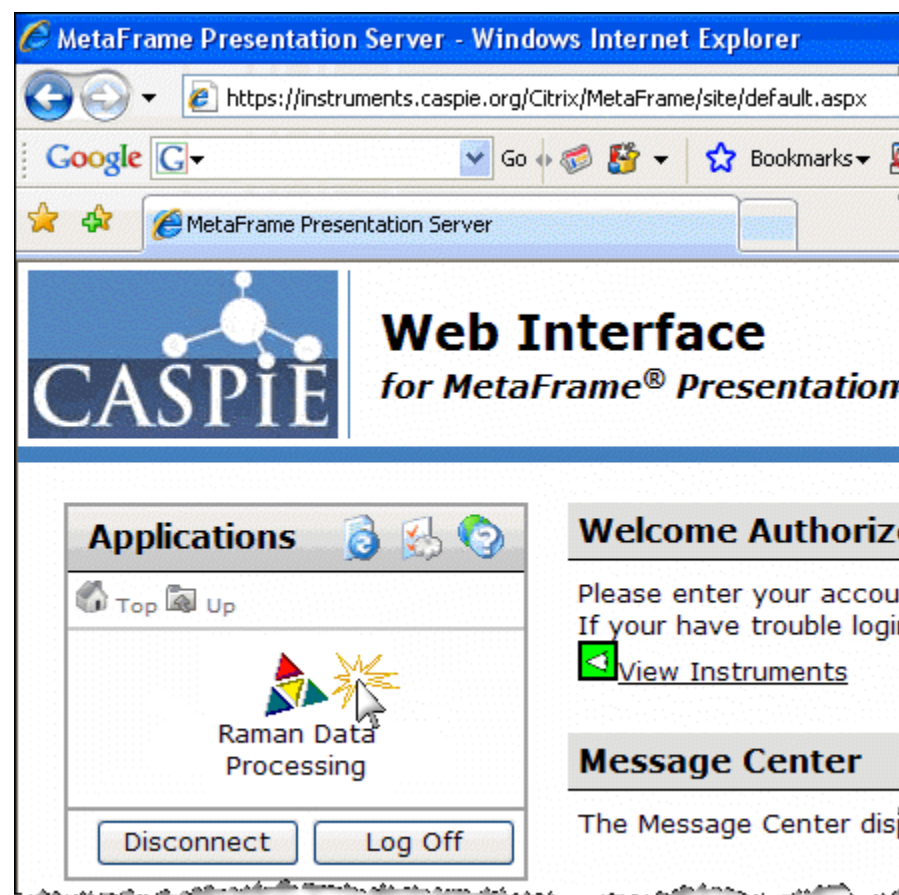
Important Note:
You must have the Citrix plugin installed on your computer to proceed!



Launch Raman Data Processing Software



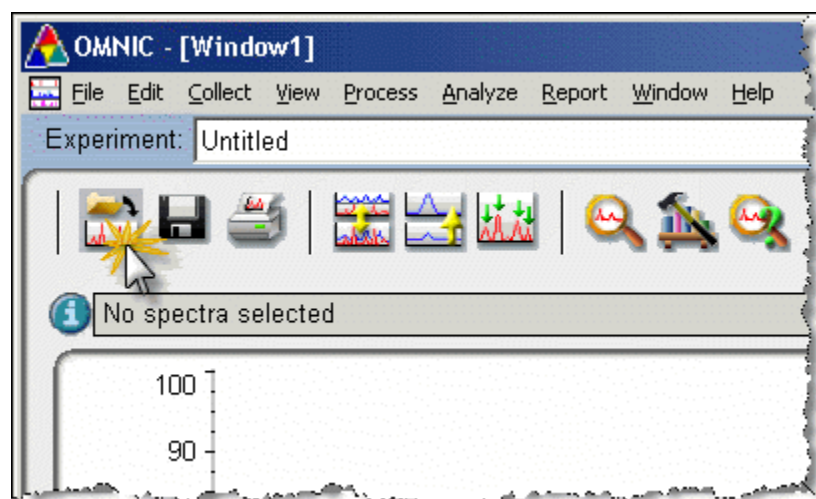
- You should see at least one icon in the 'Applications' box.
- Launch the 'Raman Data Processing' software by clicking once on the icon.
- If this icon is not present ask your TA for help.



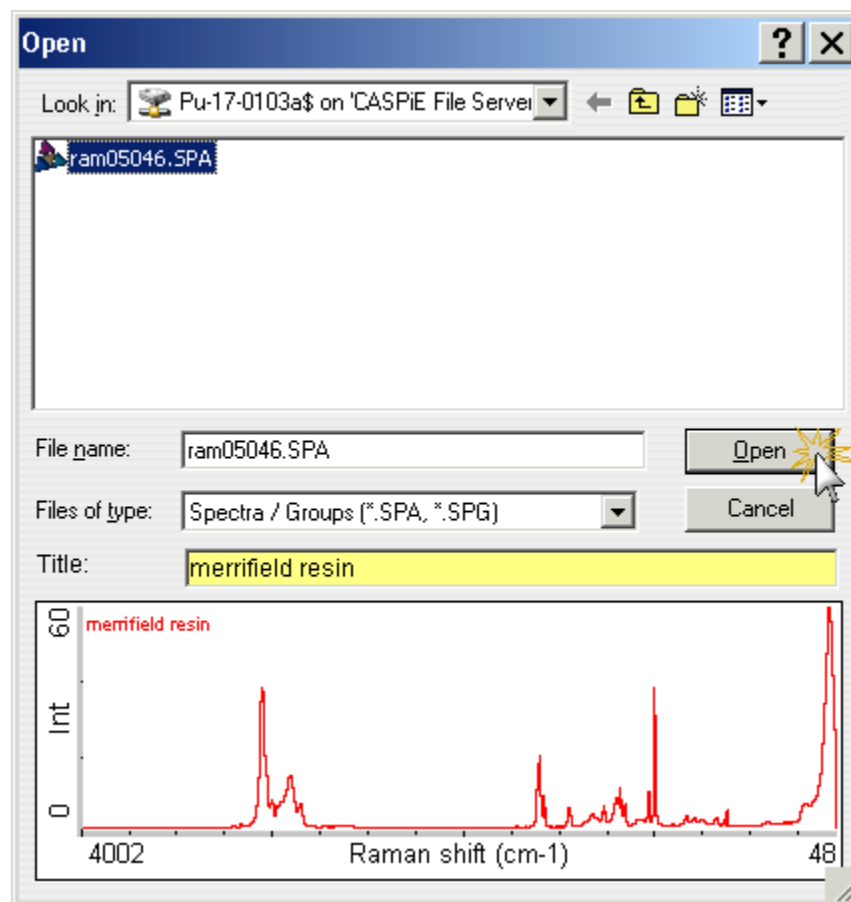
Open Data File

- Open a data file by clicking on the File Open icon (a) or selecting File | Open.
- In the Open window select your file and click open (b).

(a)

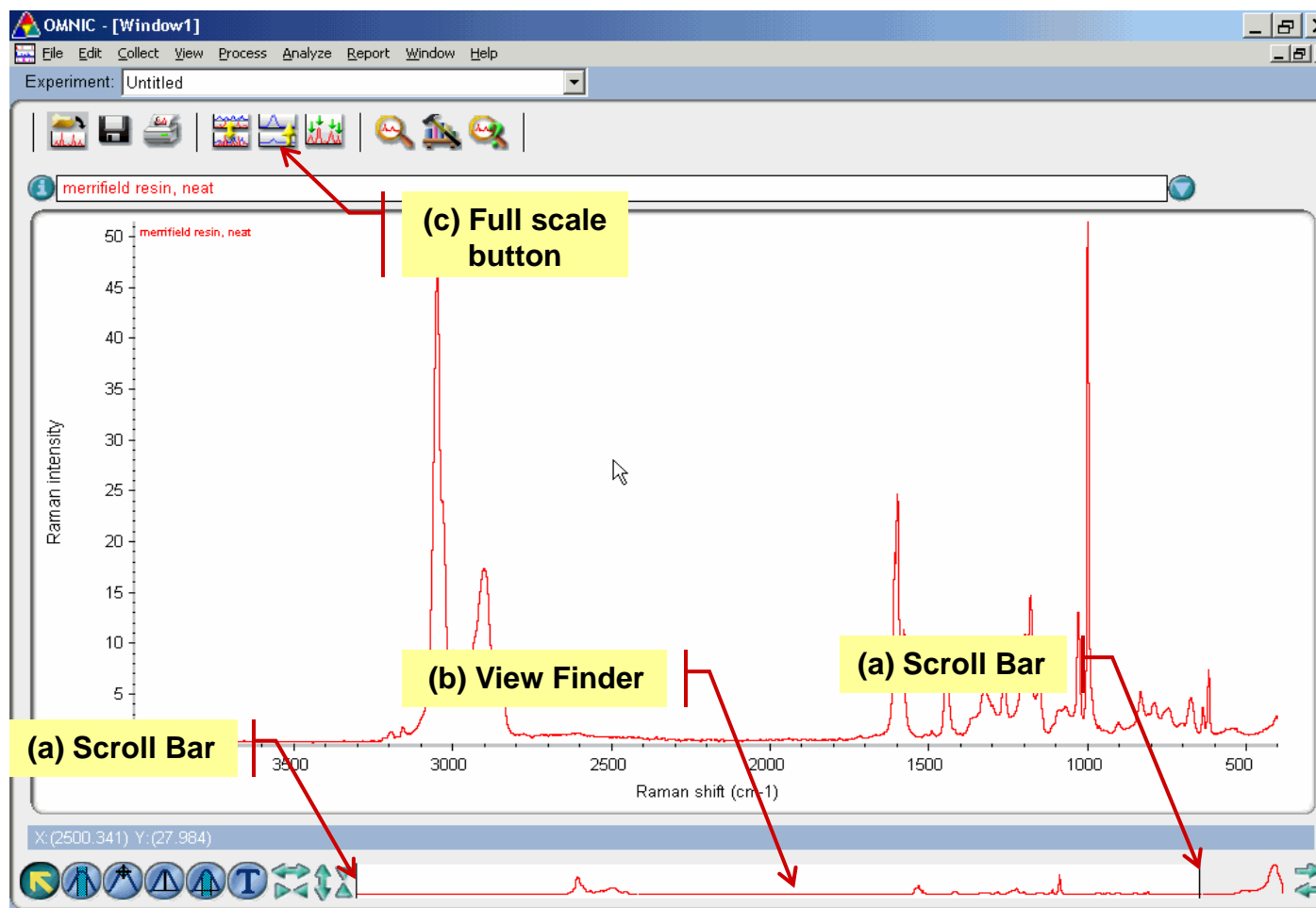


(b)



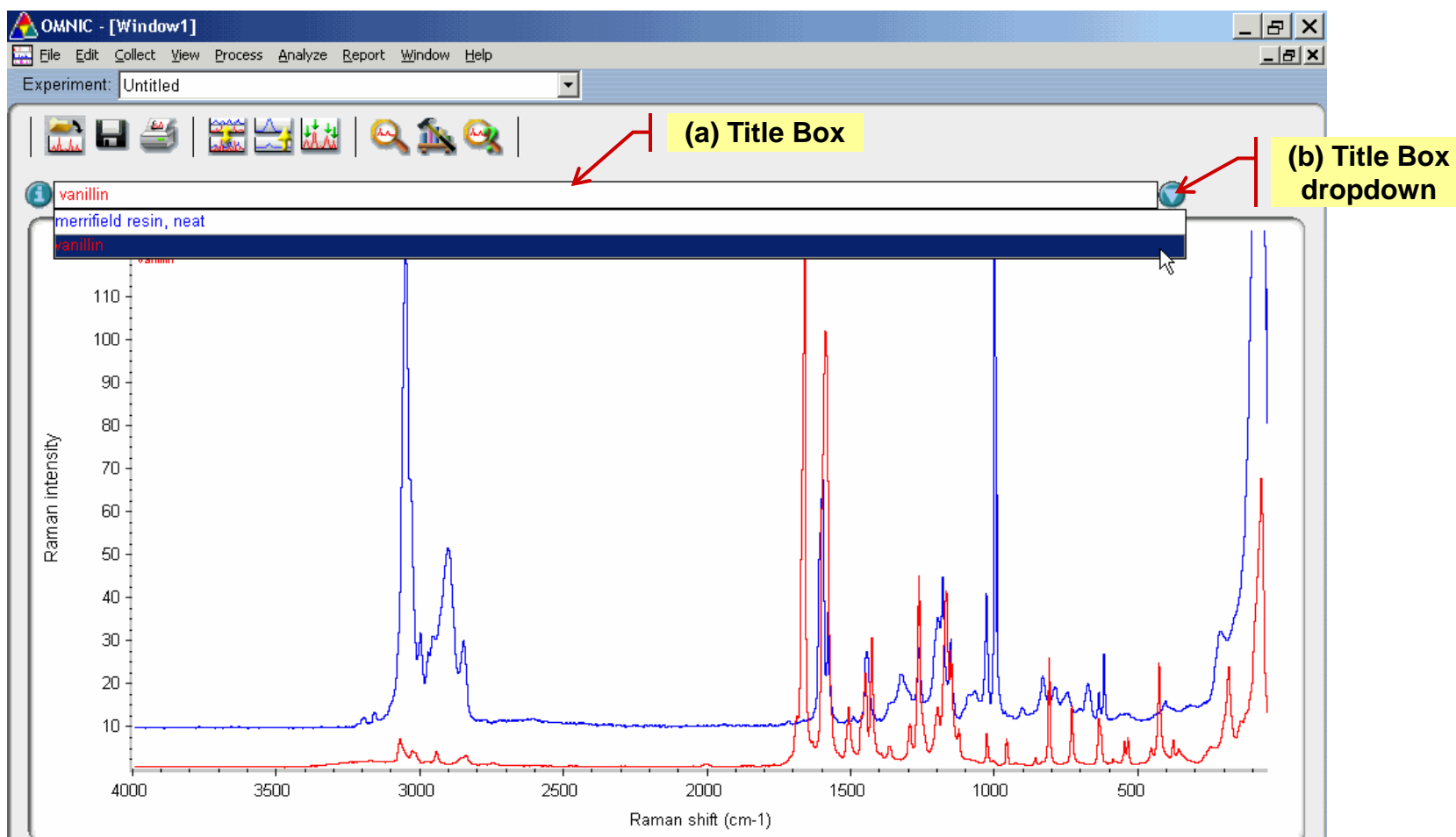
The Display Window

- To change the X-axis display select “View | Display Limits” from the menu. Enter the desired x-axis limits. Or drag the scroll bars (a) on the view finder (b).
- To autoscale the y-axis select “View | Full Scale” from the menu or use the “Full Scale” (c) button on the tool bar.



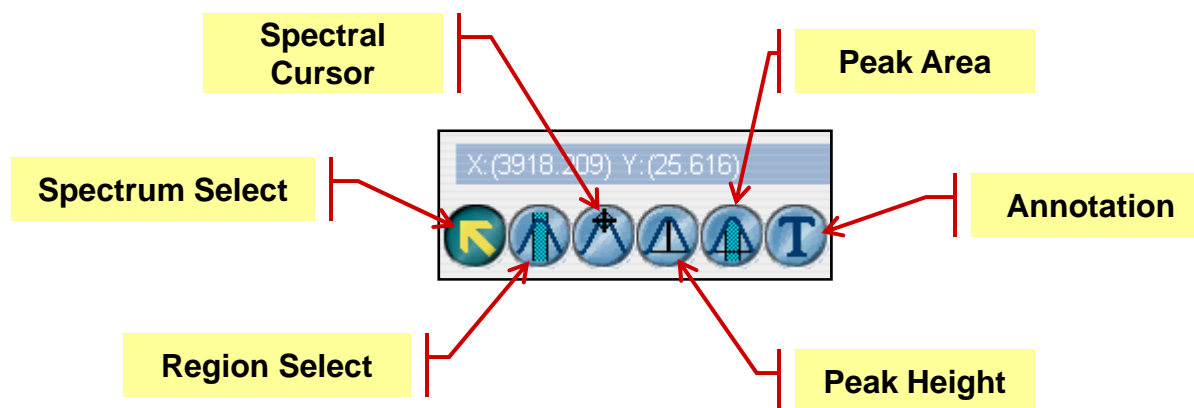
Viewing Multiple Spectra

- You may view multiple spectra in one window; just open the desired spectra into one window. The **active** spectrum is red. *The active spectrum is the one on which operations will be performed.* The active spectrum title is always displayed in the Title Box (a).
- To display a list of spectra in a window click on the arrow to the right of the Title Box (b). You can click on another title to make that spectrum active.



The Tool Palette

In the lower left corner of the OMNIC screen is the Tool Palette which contains six tools that let you select a spectrum or spectral region, display X and Y values, find the height or area of a peak and label a peak. The names and appearance of the palette tools indicate their functions. Only one tool can be used at a time. A tool remains selected until you select another.



Spectrum Select – with this tool you can select and move a spectrum in a window

Region Select – allows you to specify a spectral region on which to perform an operation such as ‘find peaks’

Spectral Cursor – when you click on a point in a spectrum the X and Y values are displayed in the readout above the palette

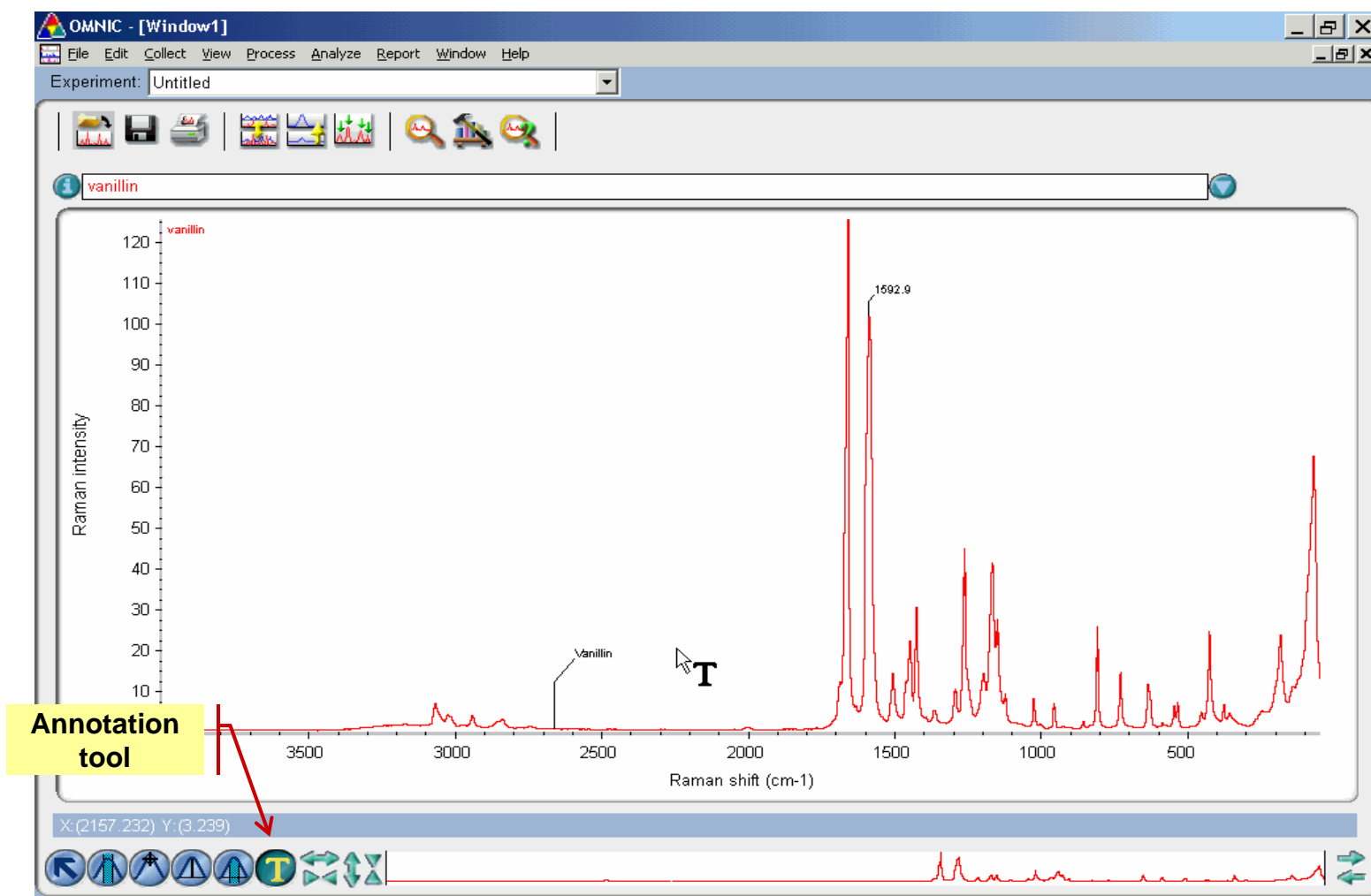
Peak Height – when you click on the top of a peak a vertical line and baseline appear; drag the baseline handles to adjust the baseline used for the peak height measurement. The results are displayed in the readout above the palette.

Peak Area – same as peak height tool except area under peak is displayed

Annotation – allows you to label peaks with their wavenumber locations or to mark a position with text

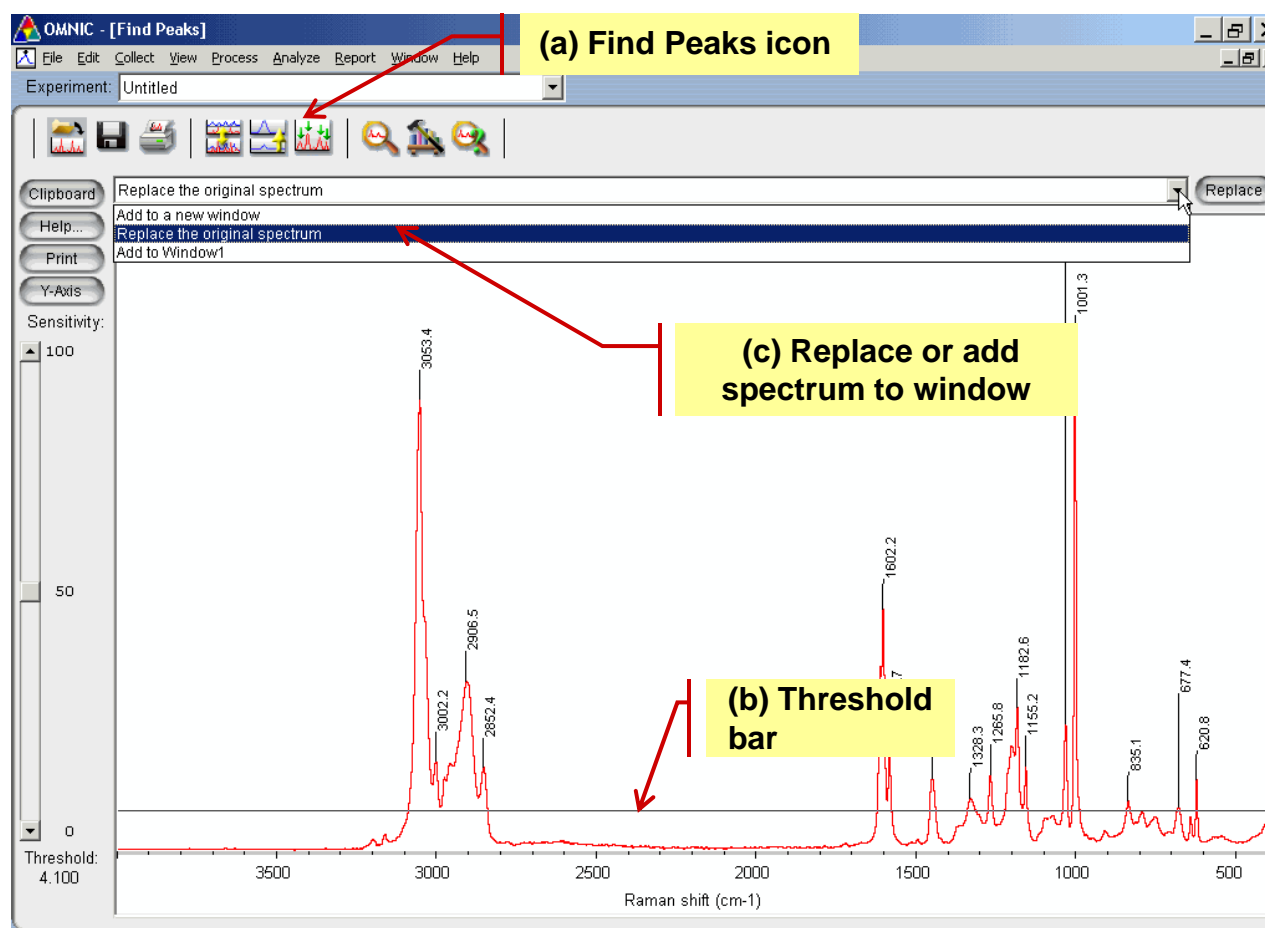
Annotation Tool

- The annotation tool allows you to attach text to a spectrum or manually mark peak positions.
- To manually mark peaks with wavenumber, click on the annotation tool, hover over the peak of interest and shift-click.



Automated Peak Finding & Labeling

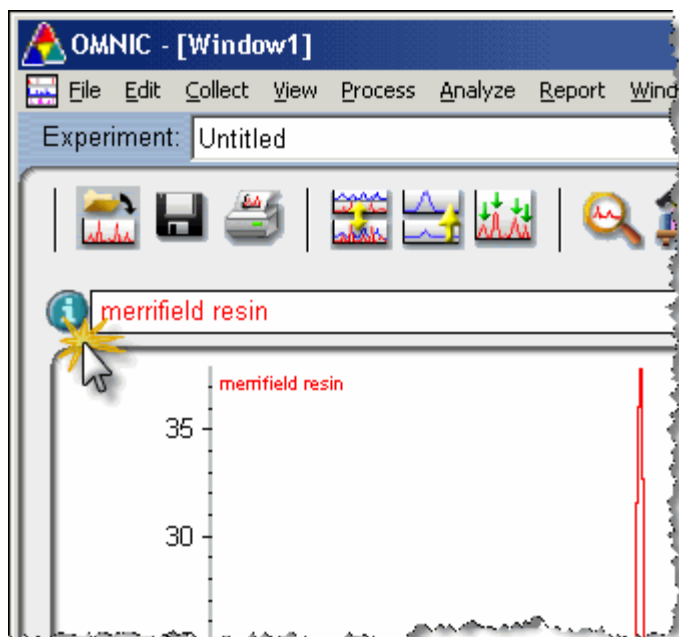
- To find and label all peaks in a spectrum click the “Find Peaks” icon (a).
- A new window will open that allows you to set the peak find threshold. Drag the threshold bar (b) to the position that picks the desired peak height.
- When you are finished, you can replace the original spectrum (c) with the marked one or you can add it to a window.



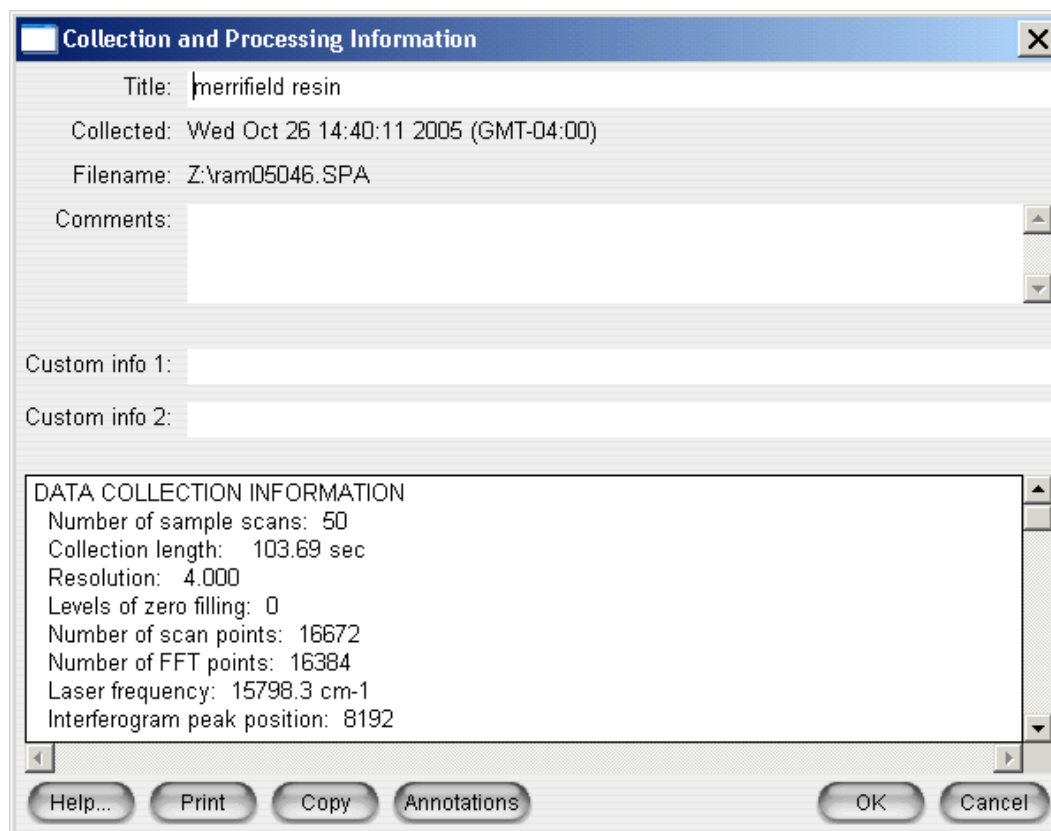
Spectrum Information

- Information about how the spectrum was collected can be displayed by clicking on the “i” button to the left of the Title Box (a).
- Anything that is done to the spectrum after collection such as a “find peaks” operation will also be displayed. You can save your own comments with a file by typing in the Comments box (b).

(a)



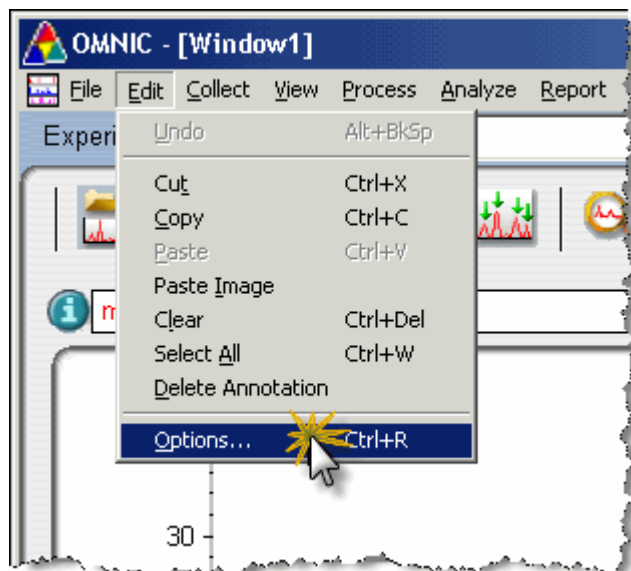
(b)



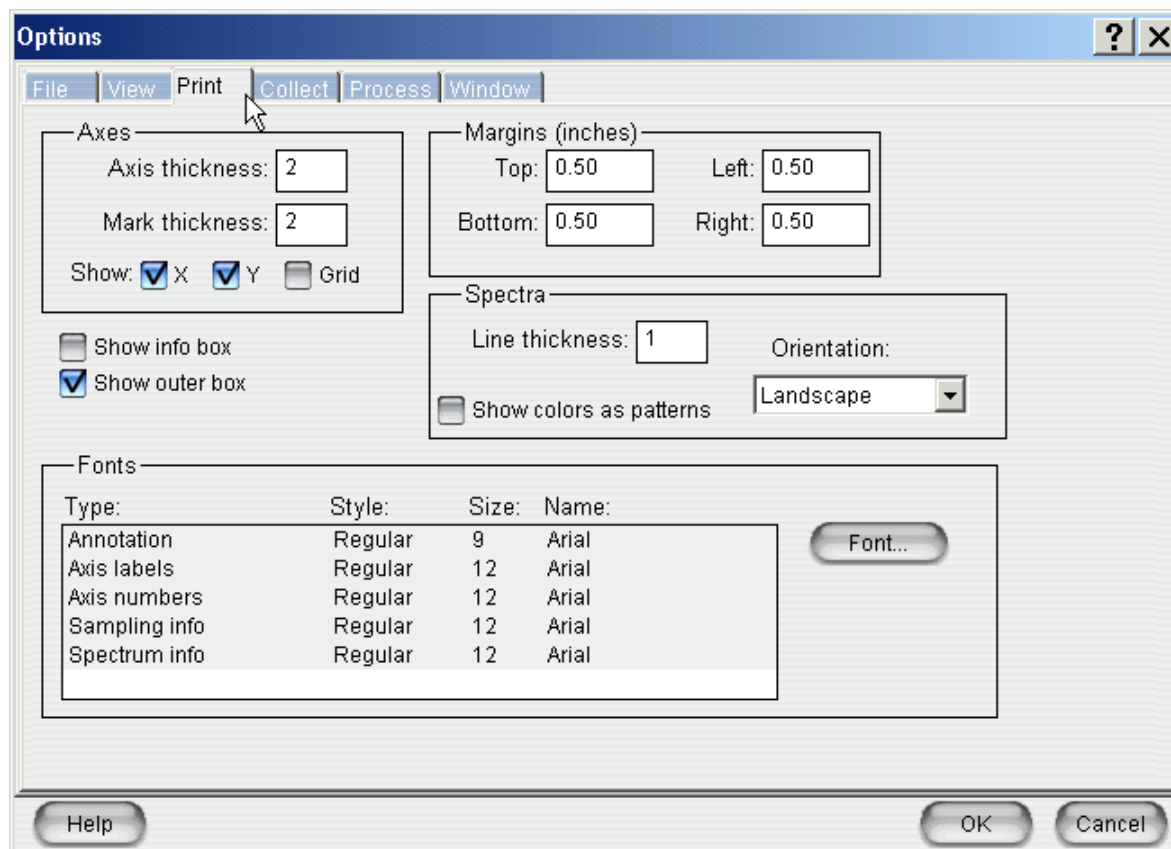
Print Options

- You can change the appearance of the printed spectrum (change line thickness, add grid, etc) by selecting “Edit| Options” from the main menu (a).
- In the Options window (b) click on the “Print” tab to view the available print options.

(a)



(b)



Exit OMNIC



- When you have finished printing be sure to exit the program.

