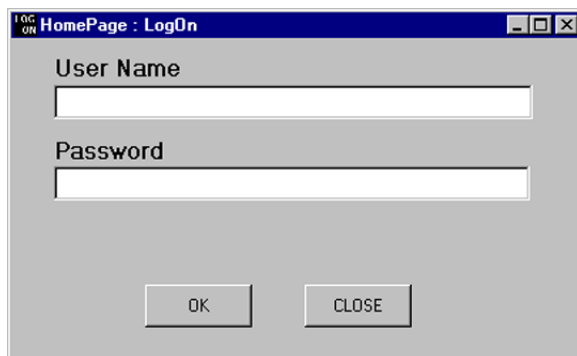


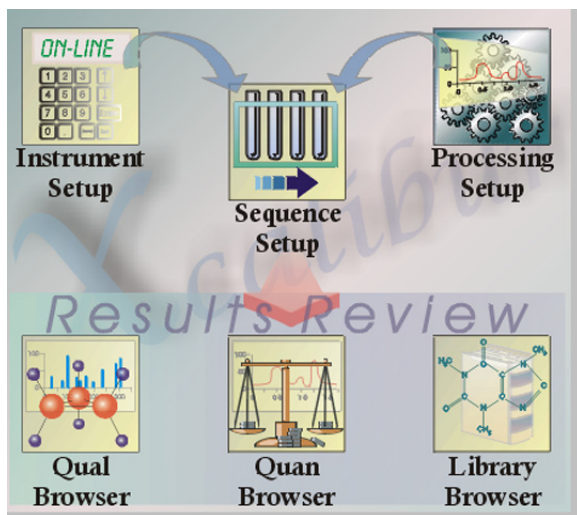
Trace GC/MS User's Booklet

- 1) Log in with your username and password.



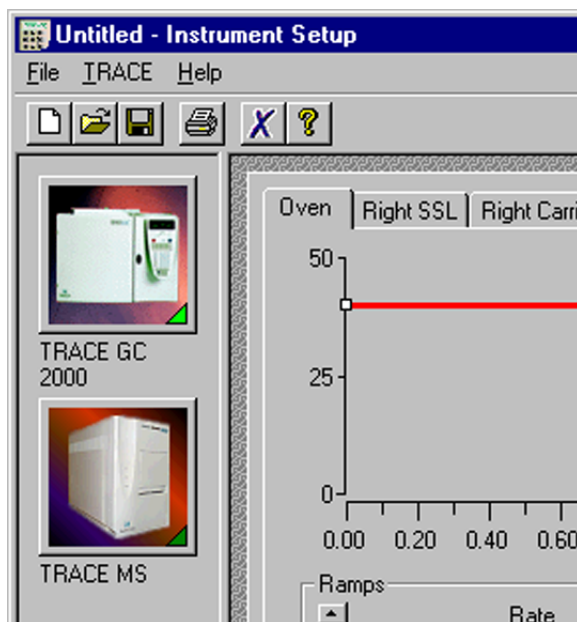
- 2) After the Xcalibur software comes up, click on the Instrument Setup icon.

Click on the Instrument Setup icon →

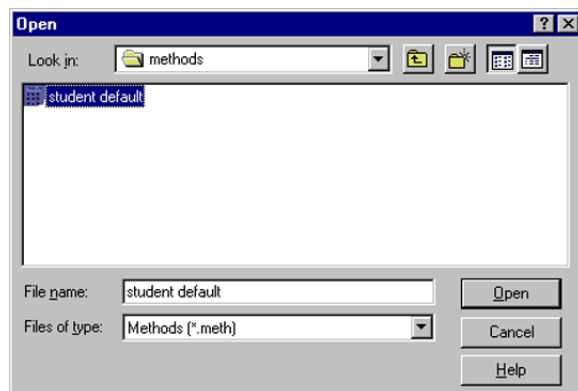


- 3) The Instrument Setup page will come up with a new, untitled method. You must open the “student default” method. Click on File, and Open, and select “student default”.

Click on the File menu, and click on Open →

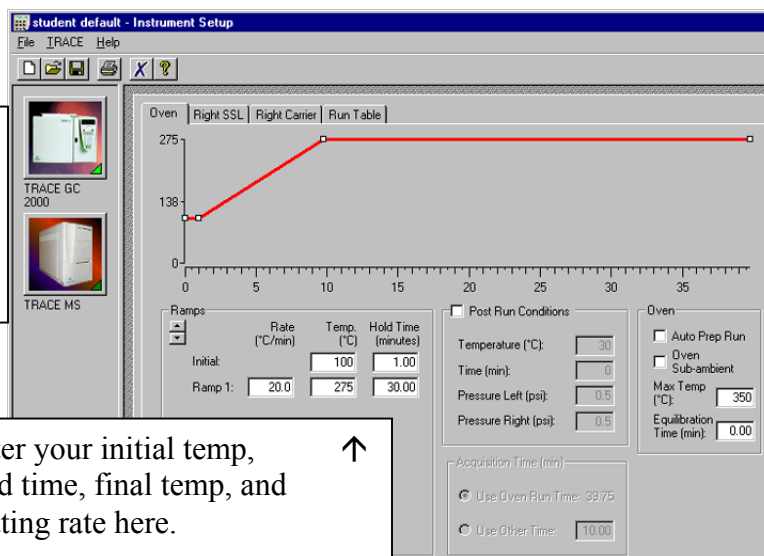


Select “student default” and click on Open →



- 4) Enter the GC conditions you want to use, such as starting temperature, hold time, final temperature, and heating rate.

Click on the TRACE → GC 2000 icon to set the GC oven parameters.

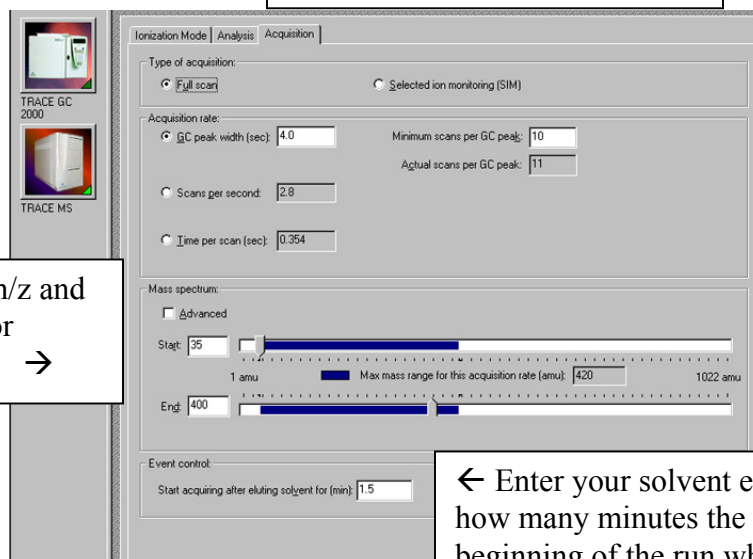


Enter your initial temp, hold time, final temp, and heating rate here. ↑

- 5) Click on the TRACE MS icon, and then the Acquisition tab, to change the starting m/z, ending m/z, and the solvent elution delay time.

↓ Click on the Acquisition tab.

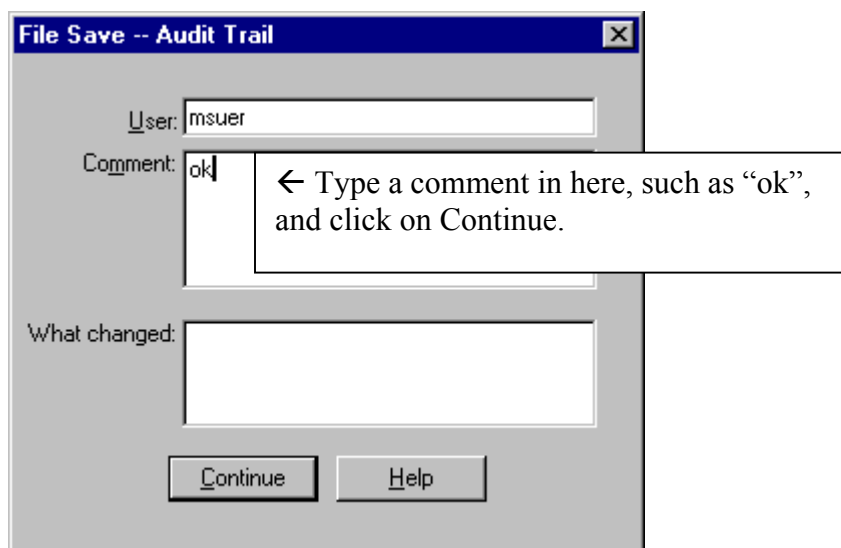
Click on the TRACE MS icon →



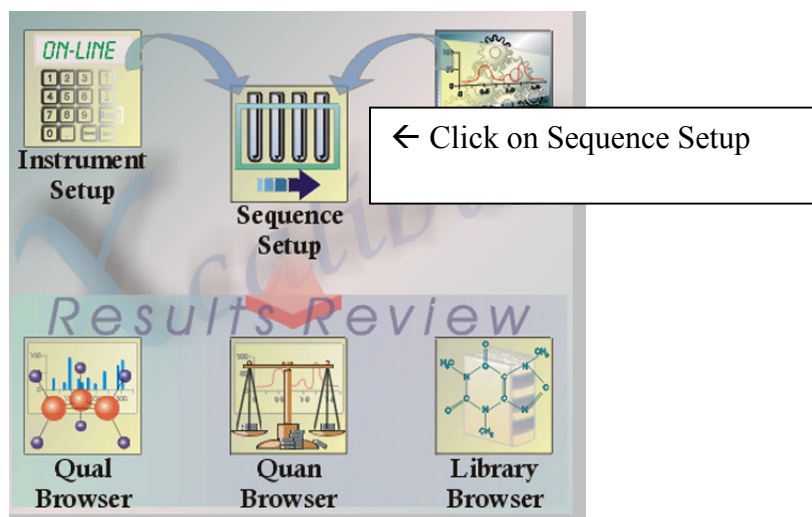
Enter your starting m/z and ending m/z values for scanning here. →

← Enter your solvent elution delay here. This is how many minutes the spectrometer is off at the beginning of the run while the solvent elutes.

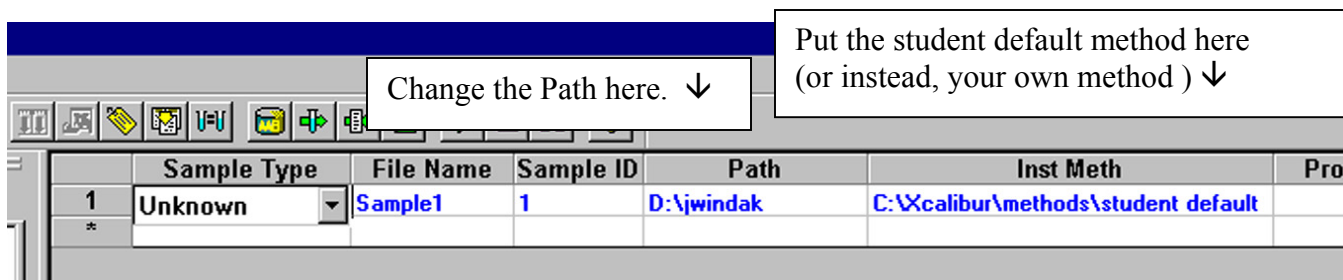
- 6) Save changes to the method, by clicking on File, and Save. **(Note: you could do a File, Save As, and give it your own name to create your own method. The important thing is to be sure to use the “student default” method as your template).** A dialog box will come up that requires you to enter something as a comment. So, just type something such as “ok”, and click on Continue.



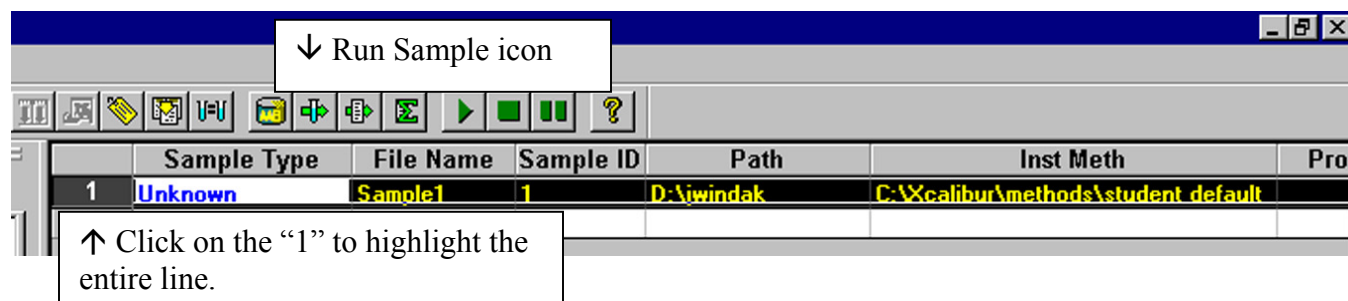
- 7) Exit from the Instrument Setup.
- 8) On the main page, click on the Sequence Setup icon. (Alternatively, you can click on the View menu, and click on Sequence Setup View).



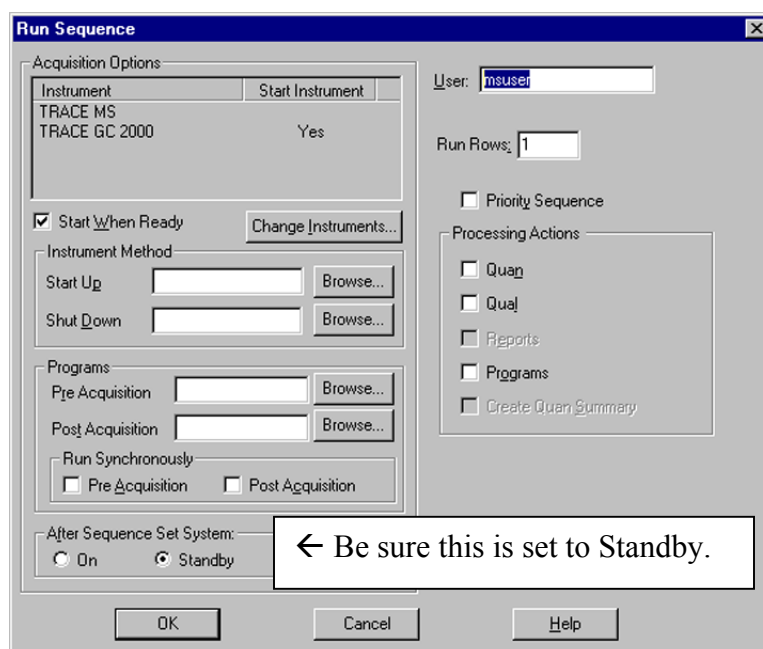
- 9) On the Sequence Setup view, fill in the information in the table for your sample. Set the Sample Type to “Unknown”. You need to enter a File Name, and set the Path by double-clicking in the Path cell. Set the “Inst Meth” to “student default”, by double-clicking in the “Inst Meth” cell, and selecting “student default” (or put your own method in here instead).



- 10) Highlight the line in the table by clicking on the “1” in front of it. Then click on the Run Sample icon on the toolbar. Alternatively, you can click on the Actions menu, and click on “Run This Sample”.



- 11) A Run Sequence dialog box comes up. Be sure that the “After Sequence Set System” is checked for “Standby”, and click on OK.



- 12) At the GC keypad, wait until the STANDBY*PREP RUN light is on steady. Then push the PREP RUN button.

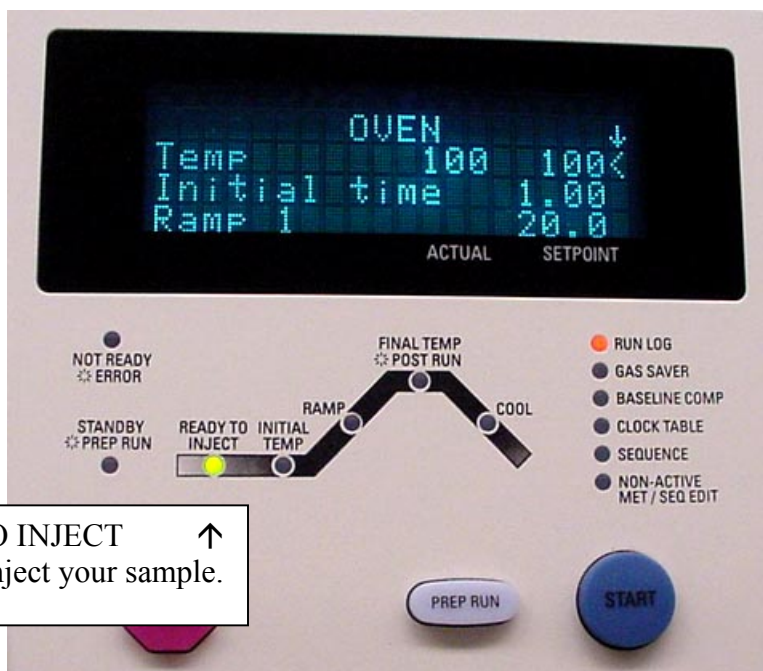
Wait until this light is on steady →



↑ Then push the PREP RUN button.

- 13) After you press the PREP RUN button, the STANDBY*PREP RUN button will flash. When the READY TO INJECT light comes on, you can inject your sample.

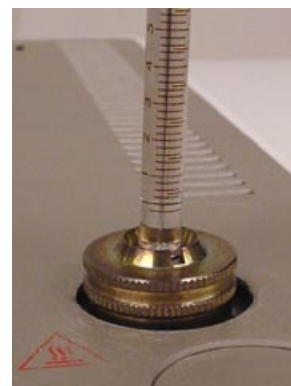
When the READY TO INJECT light is on, you may inject your sample. ↑



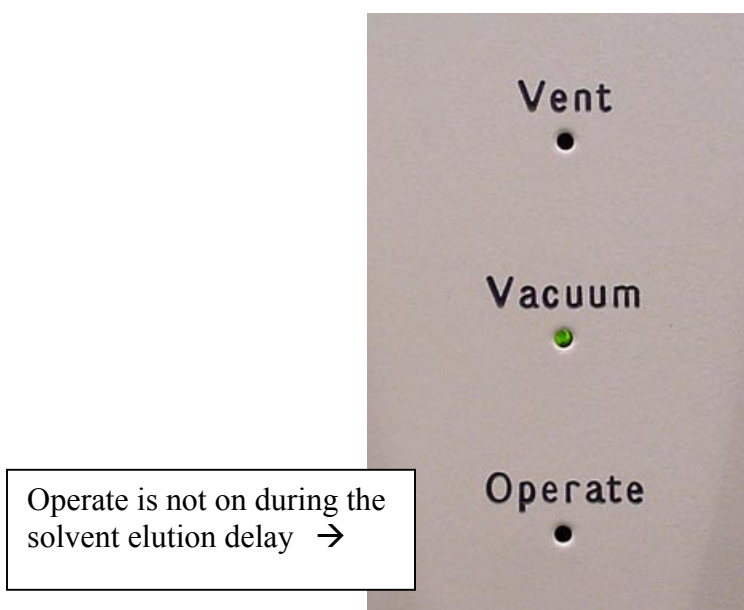
- 14) Inject your sample. **Note: Use a 10-microliter syringe only. Do not use a larger syringe.**

Please Note:

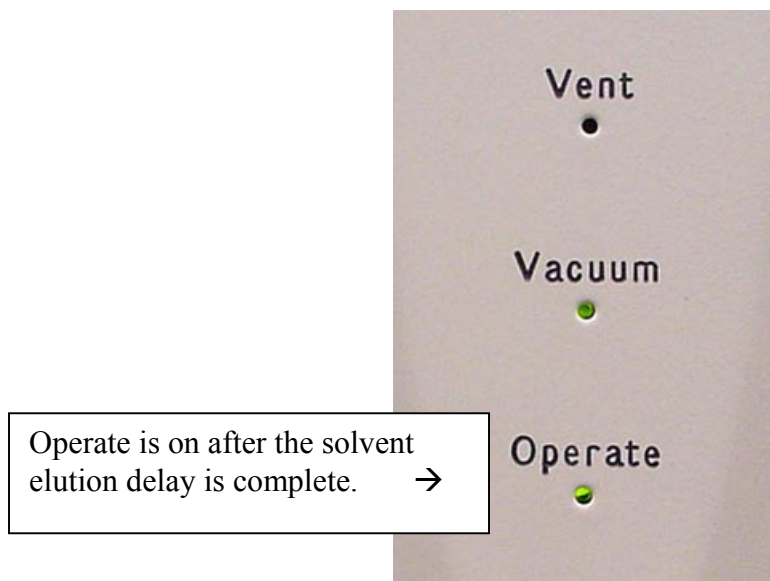
Your sample concentration must be less than 1 mg/ml for each component in the solution. You must inject 1 ul or less. If you inject samples that are too concentrated, you will damage the instrument over time. The ion source and quadrupole rods will become contaminated, causing a loss of sensitivity and mass resolution. Also, the phosphor screen detector will wear out prematurely.



- 15) During the solvent elution delay, the instrument will not be in Operate mode. You can see this on the indicator light on the front of the MS instrument.



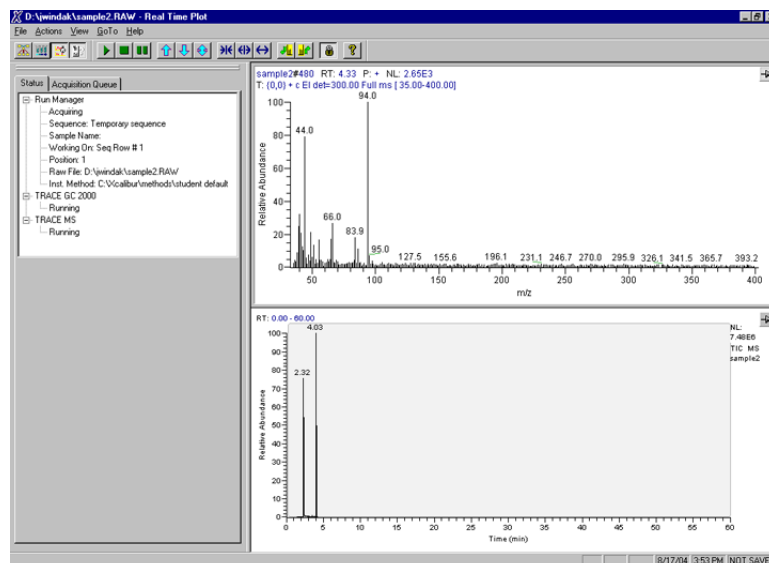
After the solvent elution delay time is complete, the instrument will automatically switch into Operate. You can see this on the front panel indicator lights.



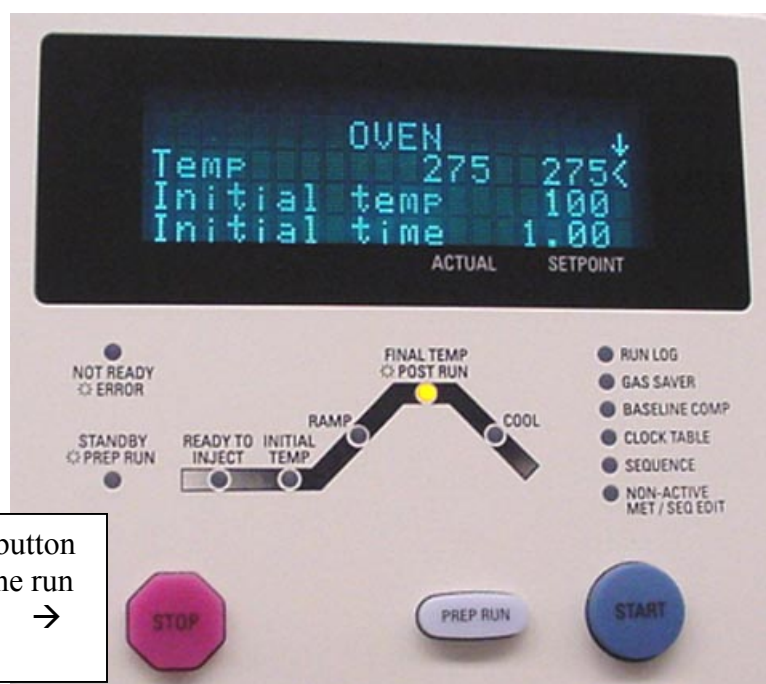
Please note:

You must set the solvent delay to a long enough time, so that the mass spectrometer is not on (not in Operate mode) while the solvent peak is eluting. Failure to do so will damage the mass spectrometer over time.

- 16) Click on the View menu, and click on Real Time Plot View, and you will see the GC chromatogram and spectra updated while the data is being acquired. For tips on using the Real Time Plot View, see the next section below.



- 17) If you want to stop the run before the acquisition time ends (the default is 60 minutes), then click on the STOP button on the GC keypad. This will stop both the GC run and the MS acquisition.



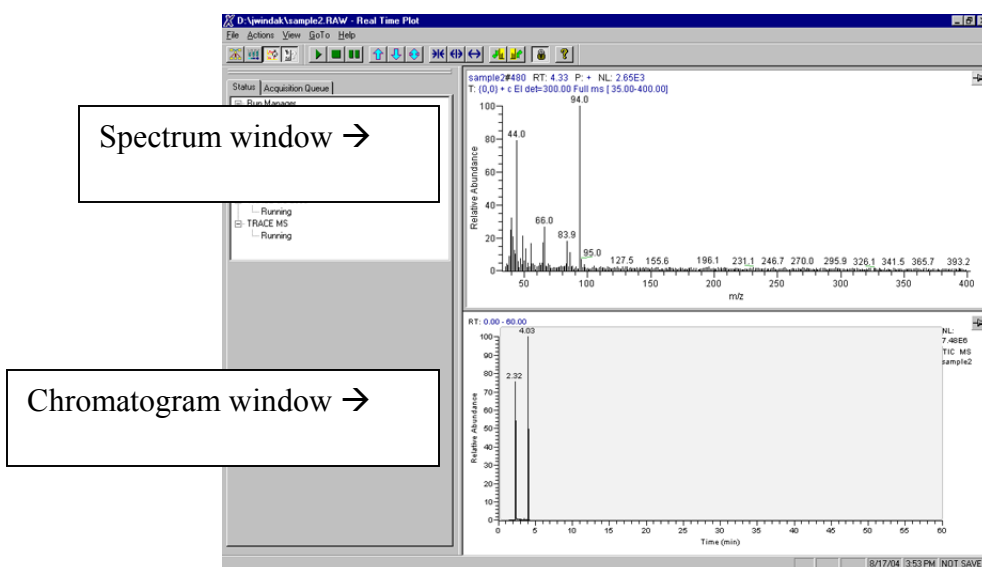
Click on the STOP button if you want to end the run before it is finished →

How to use the Real Time Plot View

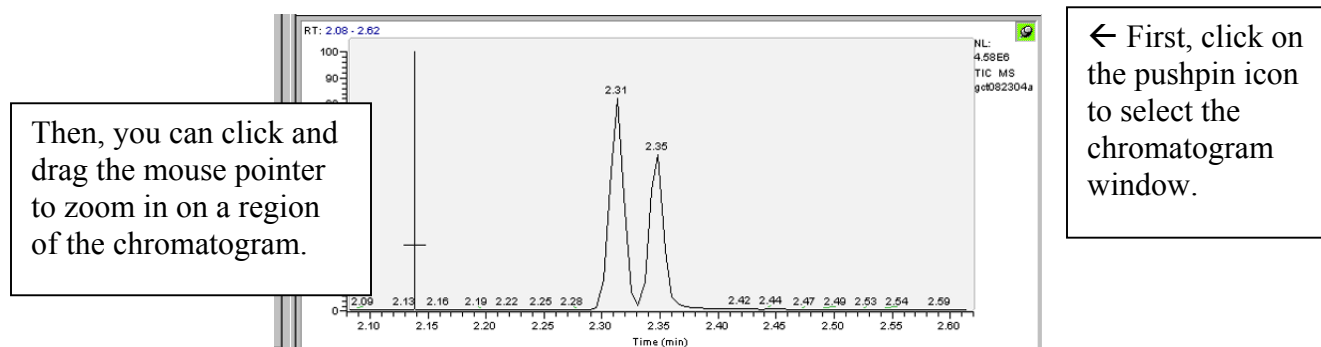
After your data acquisition is running, click on the View menu, and click on Real Time Plot View. Alternatively, you could click on the Real Time Plot View button on the toolbar.



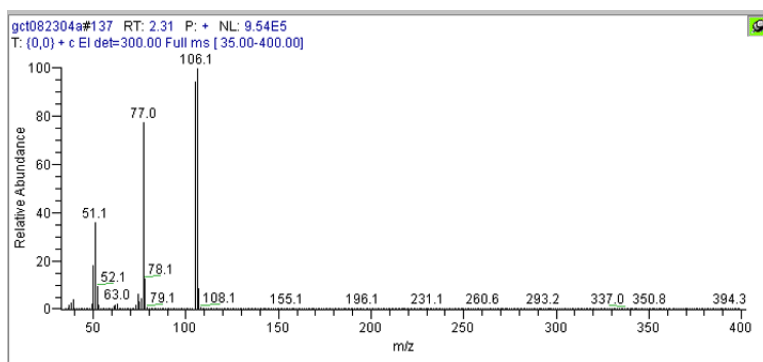
Two graphs will appear. The top graph is the mass spectrum window, and the bottom graph is the chromatogram window. They will automatically update in real time, after every mass spectrum is acquired, approximately every 0.5 seconds.



If you want to zoom into a smaller region on the chromatogram window, you must first select the chromatogram window by clicking on the pushpin icon  on the upper right side of the window.

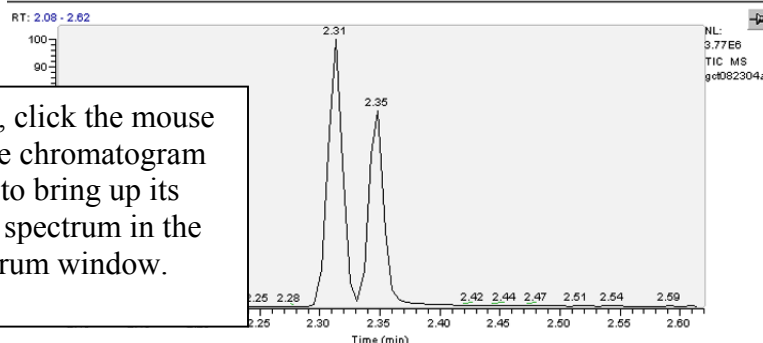


If you want to display the mass spectrum associated with a particular GC peak, you must first select the spectrum window by clicking on the pushpin icon in the upper right side of the spectrum window. Then click on a chromatogram peak to bring up its mass spectrum in the spectrum window.

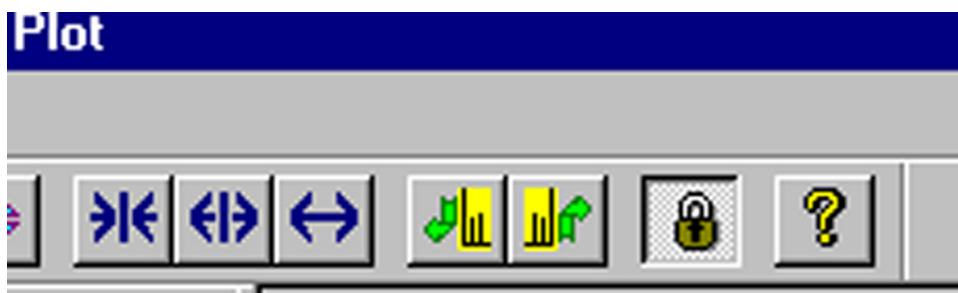


← First, click on the pushpin icon to select the spectrum window.

Then, click the mouse on the chromatogram peak to bring up its mass spectrum in the spectrum window.



While you are zoomed in on a chromatogram area, the graphs are not updating in real time. To go back to the full display that is updated in real time, you must click on the “lock display” icon on the toolbar.

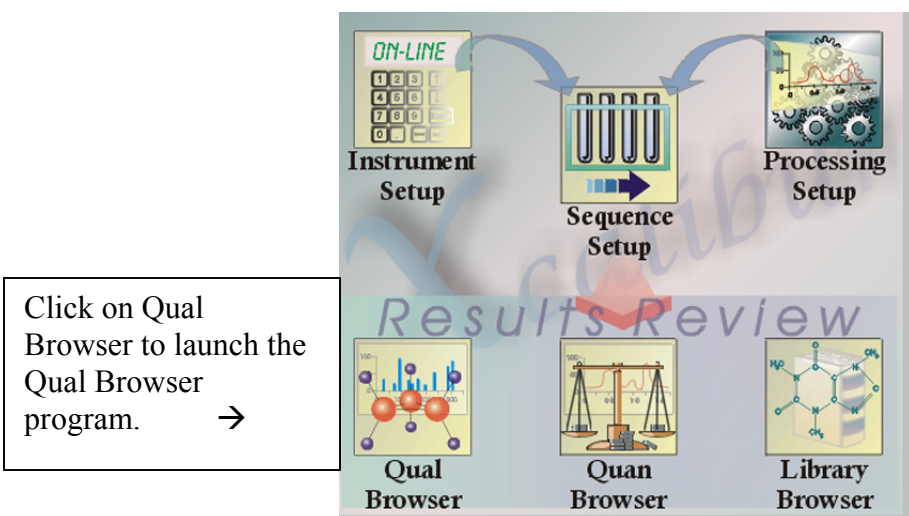
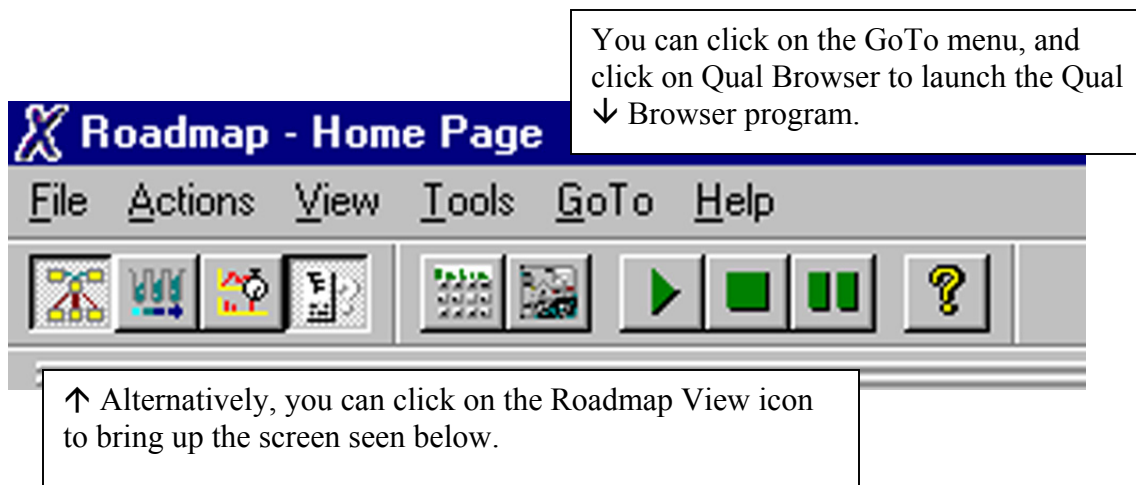


Click on the “lock display” icon on the toolbar, to make the spectrum and chromatogram windows go back to updating in real time.

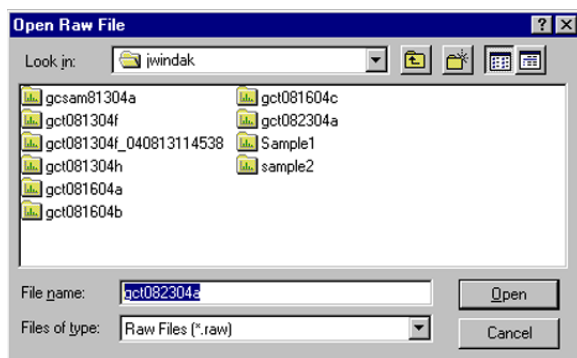


How to View Data Post Acquisition

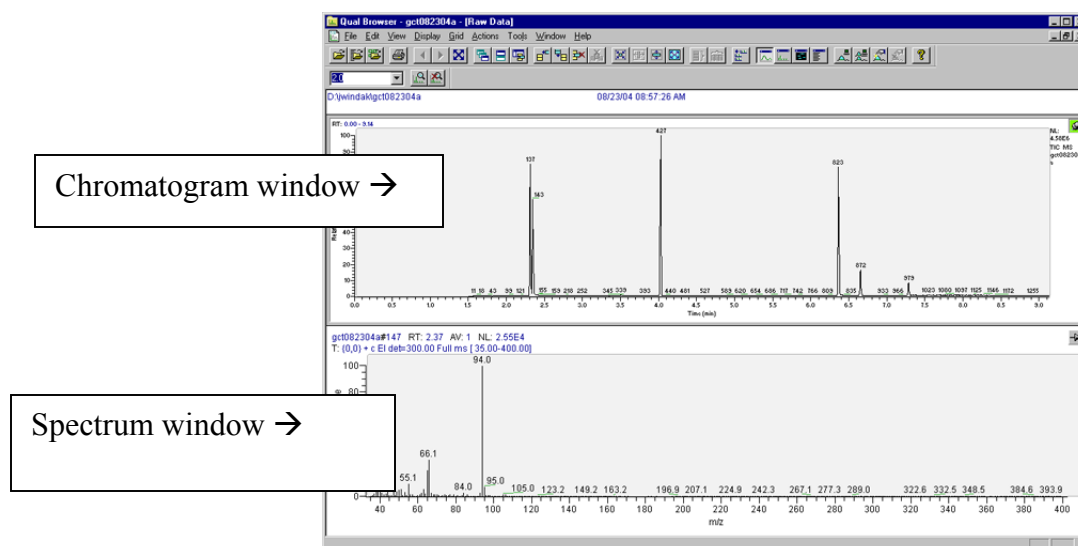
If you want to view data that has already been acquired, you need to use the Qual Browser. To do this, click on the “Go To” menu, and click on Qual Browser. Alternatively, if you click on the “Roadmap” view icon, you can then click on the Qual Browser icon.



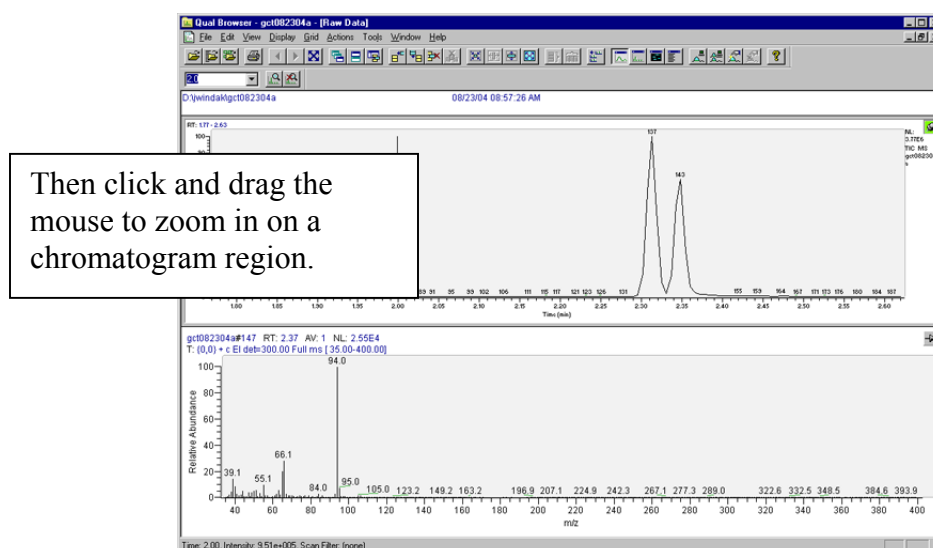
After the Qual Browser window comes up, you can open your data file by clicking on the File menu, and Open. Then browse to your datafile, and click on Open.



After your datafile is opened, a chromatogram window and a spectrum window will appear.

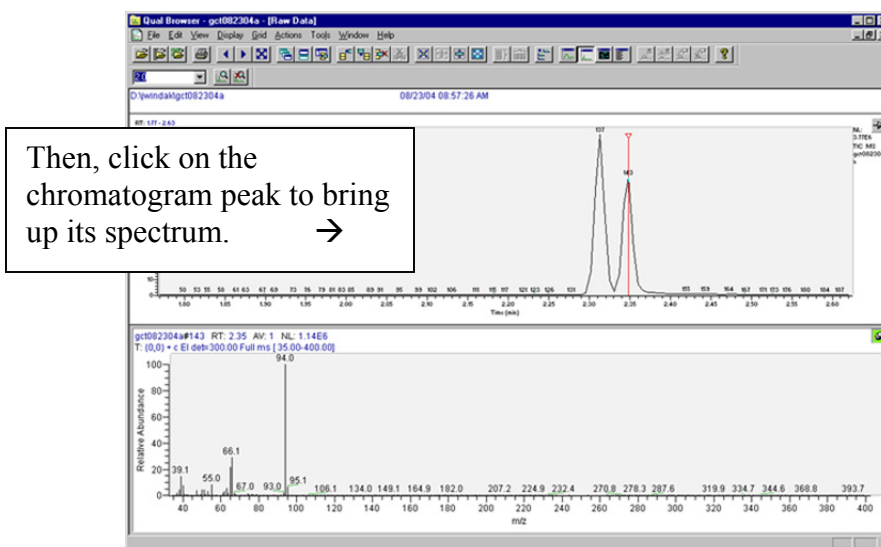


To zoom in on a region of the chromatogram, click on the pushpin icon  on the upper right side of the chromatogram window. Then click and drag to zoom in on a region.



← First, click on the pushpin icon to select the chromatogram window.

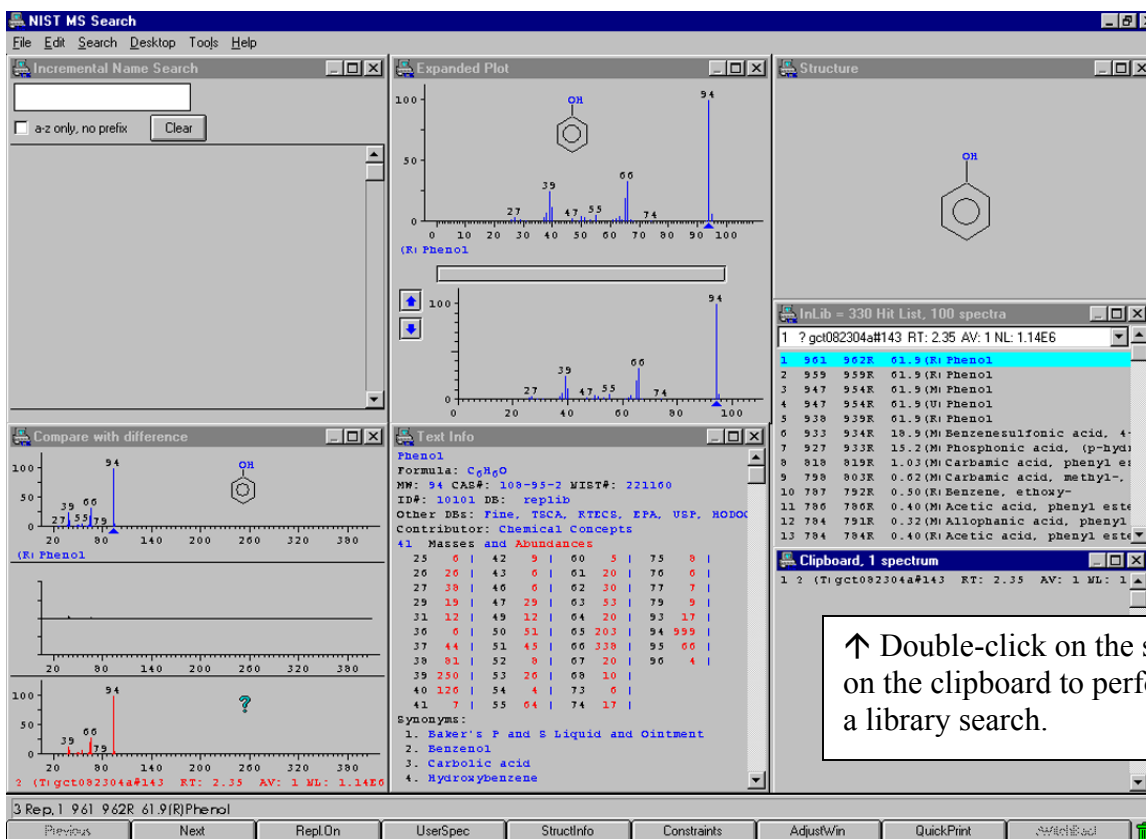
If you want to display the mass spectrum of a GC peak, click on the pushpin icon in the upper right side of the spectrum window. Then click on the chromatogram peak to bring up its spectrum.



Then, click on the chromatogram peak to bring up its spectrum. →

← First, click on the pushpin icon on the spectrum window.

If you want to search the NIST library, right click the spectrum window, and then left-click on “Library”, and then left-click on “Export to Library Browser”. This will take you into the NIST library program. Once you are in NIST, double-click the scan on the clipboard to do a library search on it.



↑ Double-click on the scan on the clipboard to perform a library search.

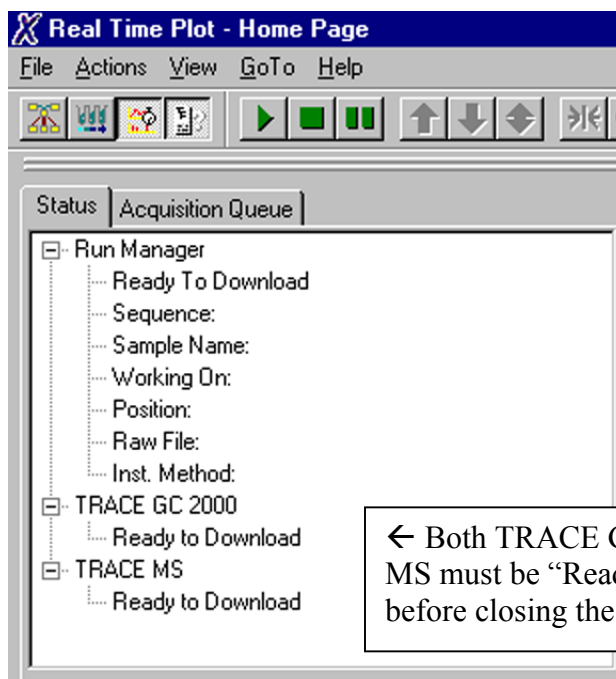
How to Shut Down When You are Finished

- 1) Close the NIST library window if it is open.
- 2) Close the Qual Browser window if it is open.
- 3) If an acquisition is in progress, stop it by pushing the STOP button on the GC keypad.



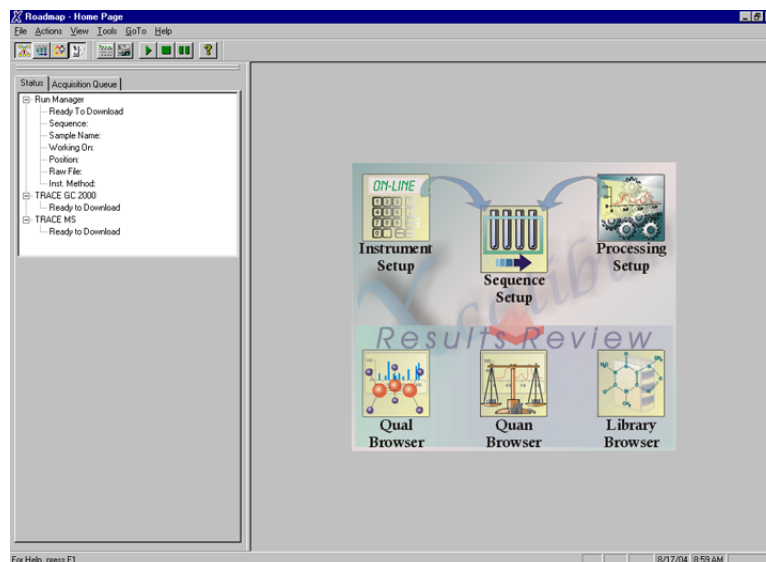
Click on the STOP → button to stop an acquisition if an acquisition is still running.

- 4) On the main page, look at the status window, and look at TRACE GC 2000, and TRACE MS. After you stop the run, they will both say "Post Acquisition", and then they will both say "Ready to Download". Be sure to wait until they say "Ready to Download" before closing the main Xcalibur window.

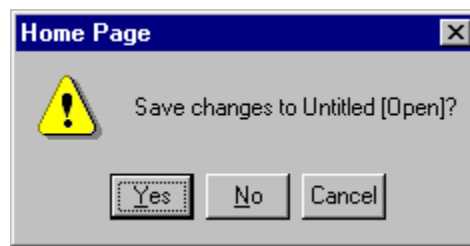


← Both TRACE GC 2000 & TRACE MS must be "Ready to Download" before closing the main page.

- 5) Finally, close the main page window. It will ask you whether you want to save changes to Untitled. Click on No. This will then log you out of the system.



← Click on the  icon to close the main page.



↑ Click on No to save changes to Untitled (Open)

When you see this login window, you know you are completely logged off.

