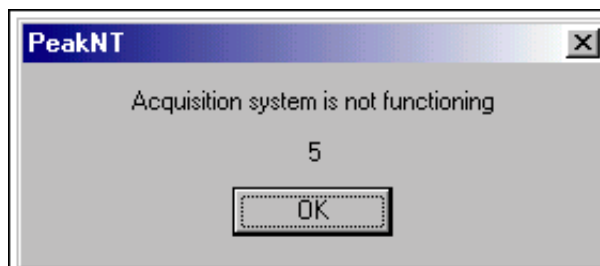




## Launching PeakSimple 2000

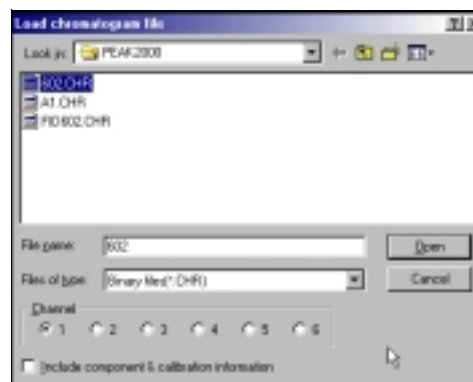
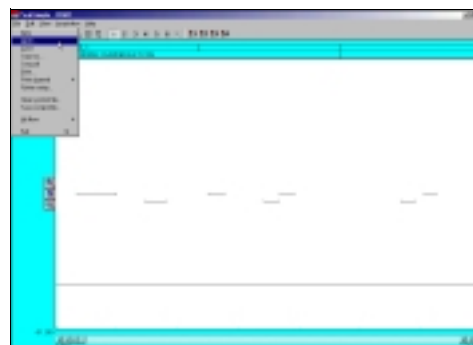
1. Click on the windows **Start** button in the bottom left-hand corner of the screen. Select **Programs** and then **PeakSimple** from the list of program groups on the screen and then click on **PeakSimple**.
2. This will launch PeakSimple and initialize the data acquisition system.
3. If PeakSimple comes up with an error message stating "Acquisition system is not functioning" with a countdown timer, it is indicating that there is a communication problem between the computer and the data system or that the data system and the hardware is not connected. Click **OK** to continue working with PeakSimple.
4. Most of the commands and options in PeakSimple are equipped with tool tips that will automatically pop up to display useful information when the mouse cursor is held over a command. To turn off the tool tips deselect the tool tips option in the Help menu.



Click this button to jump to the integration parameters screen. This is sometimes useful when reviewing the results data. For example, if the area spec caused some peaks to be skipped, you can jump right to the integration parameters and adjust the area spec number.

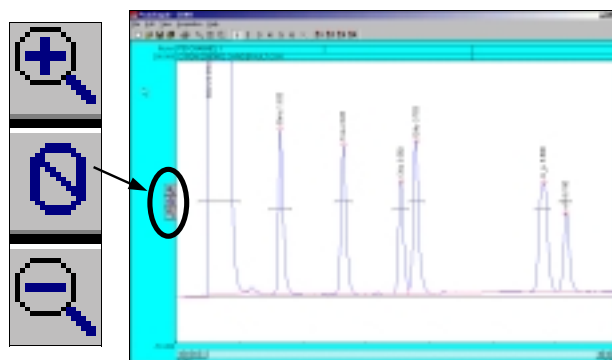
## Opening a PeakSimple Data File

1. To open a PeakSimple data file or chromatogram, begin by selecting **File** in the PeakSimple menu bar and then choose **Open...** from the set of options.
2. The Load Chromatogram File window is now open. The PeakSimple software includes a number of sample chromatogram data files that can be opened, displayed, and manipulated. One file, 602.CHR, will be used throughout the rest of the tutorial. Select file **602.CHR** from the PeakSimple directory, choose **Channel 1** as a destination channel, and then select **Open** to load the file.



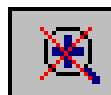
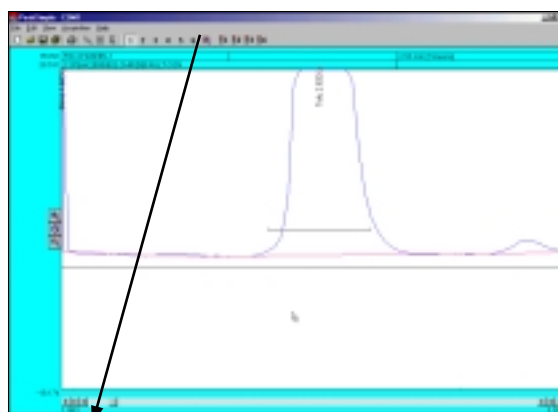
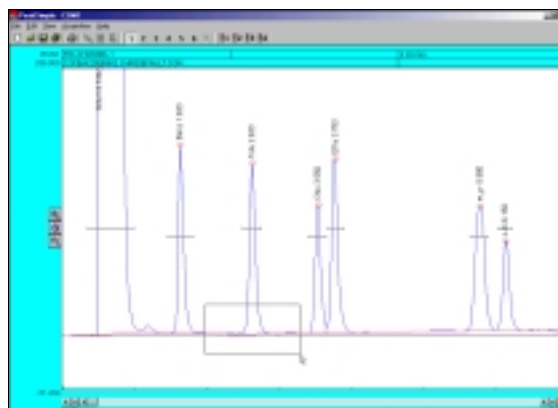
## Adjusting Display Limits

1. To adjust the display limits of a chromatogram click on either the + magnifying glass icon or the - magnifying glass icon to the left of the chromatogram. This will increase or decrease the limits by a factor of two each time you click on the icons.
2. After opening chromatogram 602.CHR, practice making the display limits smaller but the peaks larger by clicking the + magnifying glass icon.
3. Practice making the display limits larger but the peaks smaller by clicking on the - magnifying glass icon.



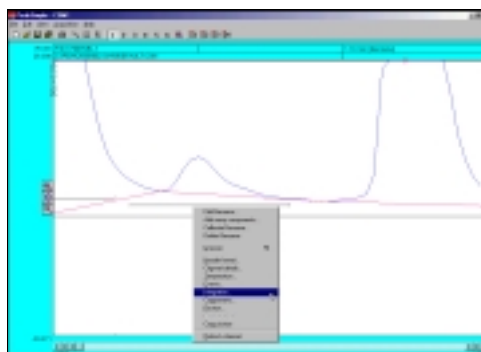
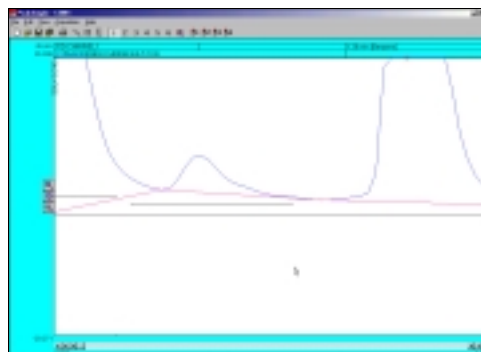
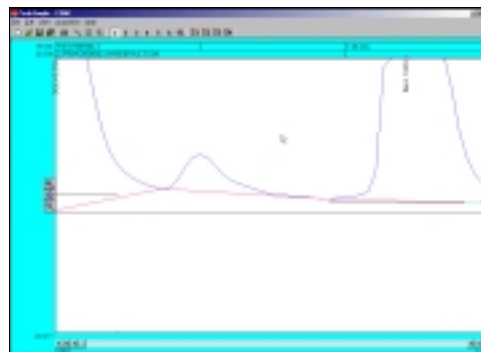
## Zooming

1. To zoom in on a specific part of a PeakSimple chromatogram, click and hold the left mouse button and drag it over the desired area.
2. After opening chromatogram 602.CHR hold the left mouse button and drag it over the base of the toluene peak. Let go of the mouse button and there will be a larger view of the area that was selected.
3. To return to the original display limits of the chromatogram and unzoom the area selected press **F6** or select the unzoom icon located in the PeakSimple toolbar at the top of the screen.



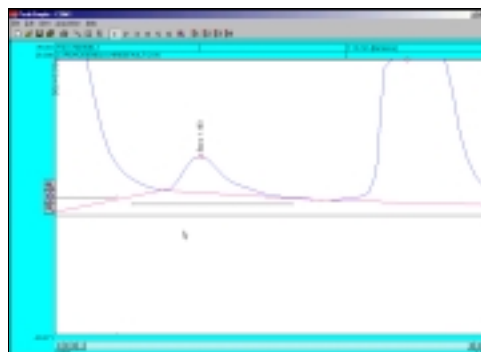
## Dragging Retention Windows

1. To drag a retention window bar place the mouse cursor on the bar until a double sided arrow pops up. Click on the left mouse button and hold and then drag the retention window bar to its desired place.
2. After opening the chromatogram 602.CHR zoom in on the benzene peak and the smaller peak to its left. Locate the benzene retention window bar and drag it over to the smaller unnamed peak to the left of the benzene. Because this is a small peak it is not immediately recognized.
3. Right click on the chromatogram over the unnamed peak and select **Integration** from the resulting menu.
4. From the integration window locate the **Area Reject** dialogue box, erase the 100.0 in the box, and add the number **10.0** to the dialogue box. Click **OK** and the integration window will exit.
5. Press the **Enter** or **Return** key on your keyboard and the smaller peak will now be recognized as Benzene.



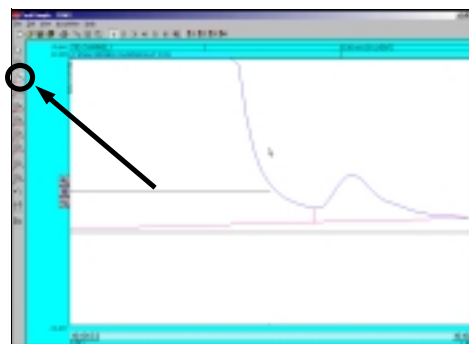
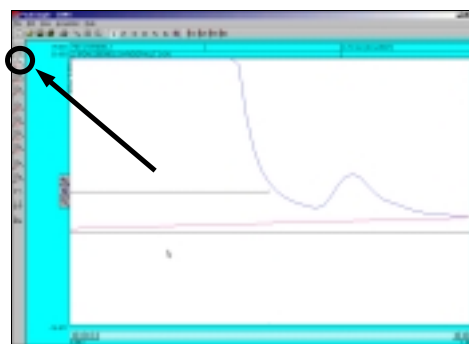
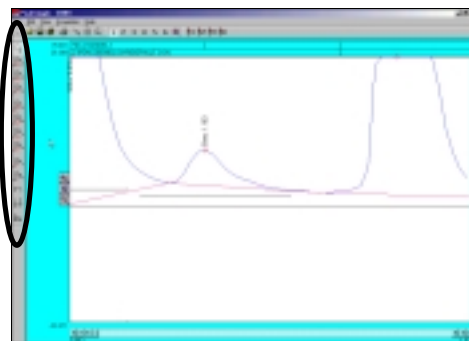
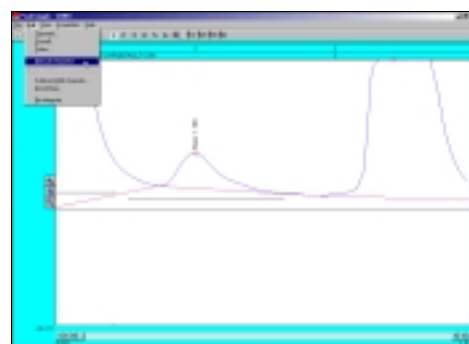
Channel 1 integration

Peak detection sensitivity	Spike channel	Merge results from channels
Eval: 95.00 %	<input type="checkbox"/> None	<input type="checkbox"/> 2
Base line: 50.00 %	<input type="checkbox"/> 2	<input type="checkbox"/> 3
Area reject: 10.0	<input type="checkbox"/> 3	<input type="checkbox"/> 4
	<input type="checkbox"/> 4	<input type="checkbox"/> 5
	<input type="checkbox"/> 5	<input type="checkbox"/> 6
	<input type="checkbox"/> 6	
Standard weight: 1.000	Saddle weight: 1.000	
OK		Cancel

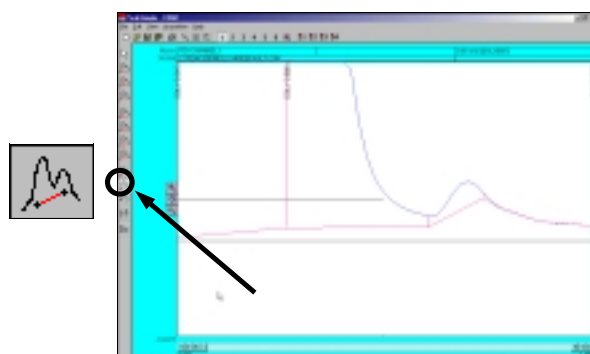
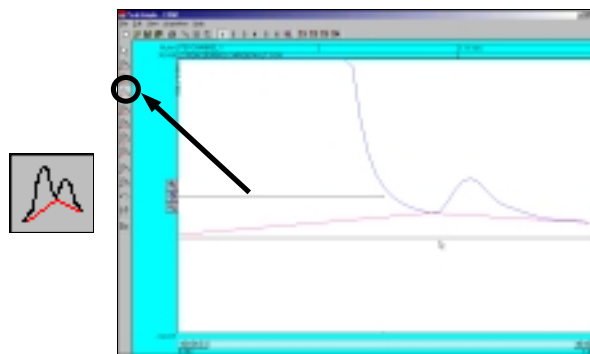


## Manual Integration

1. To manually adjust the integration baseline and peak separation in a chromatogram use the manual integration toolbar provided by PeakSimple. To open up the manual integration toolbar select **Edit** in the PeakSimple menu bar and then click on the **Manual Integration** option. The manual integration toolbar will now appear to the left of the chromatograph.
2. The manual integration toolbar contains nine types of manual integration options. Four of the most commonly used options are **None** integration, **Drop** integration, **Based** integration, and **Rubber Band** integration.
3. To make a baseline ignore a peak use the None integration tool. After opening chromatogram 602.CHR and the manual integration toolbar, zoom in on the baseline of the solvent peak and the smaller unrecognized peak immediately to its right. Click on the **None** integration tool in the manual integration toolbar with the mouse cursor and then click on the valley between the two peaks where they meet the baseline. The area of the small peak is now added to the solvent peak.
4. To undo the changes made to a chromatogram at any time simply click on the **Undo** integration tool in the manual integration toolbar. After selecting this tool all integration changes made to the chromatogram will be undone.
5. Click on the **Undo** tool with your mouse cursor and select the **Drop** integration tool to enable the dropping of the baseline below the between the two peaks. After selecting the Drop tool click where the valley of the peaks meet the baseline with the cursor. The baseline should now be dropped below the base of the peaks and a line should extend from it to the baseline.

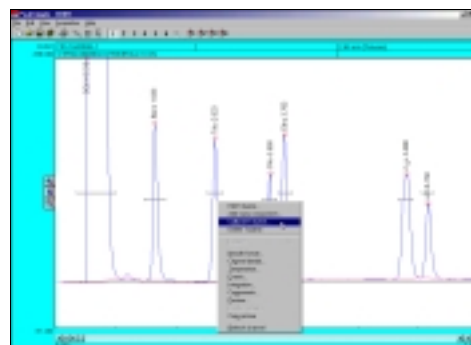


- After the manual integration between the two peaks is dropped use the **Based** integration tool to raise the baseline to the valley between the peaks. Once the Based integration tool is selected, click on the valley between the solvent peak and the smaller peak to its right with the mouse cursor. The baseline will now extend up to meet the valley of the two peaks.
- Once again click on the **Undo** tool in the manual integration toolbar to remove all changes done to the chromatogram. Select the **Rubber Band** integration tool to manually draw a baseline. Once the Rubber Band tool is selected take the mouse cursor and click on a part of the baseline. While holding down the left mouse button extend the line to another part of the baseline further to the right of the starting point and let go of the mouse button. The base line will now be drawn according to the line that was drawn using the Rubber Band integration tool.



## Calibration

- To turn the raw area of a peak into a real-world number the peak first needs to be calibrated. To calibrate the Toluene peak in chromatogram 602.CHR, open up the file and then right click using the mouse on the Toluene peak. After right clicking on Toluene select **Calibrate Toluene** from the resulting menu.
- From the Recalibration level window click on the third level radio button **3 (100.000)** and then select **OK** with your mouse cursor.

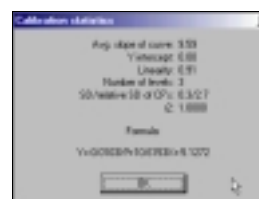
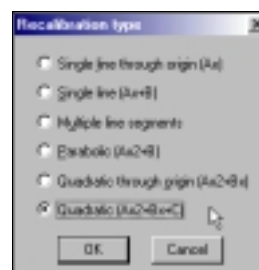
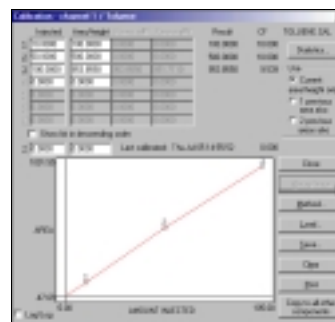


**Recalibration level** [X]

Peak: Toluene  
 Time: 2.633  
 Area: 953.855

1 (10.000)  
 2 (50.000)  
 3 (100.000)  
 4 (2.000)  
 5 (2.000)  
 6 (2.000)  
 7 (2.000)

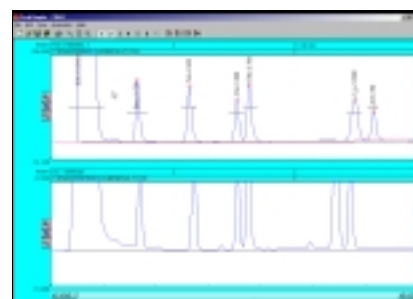
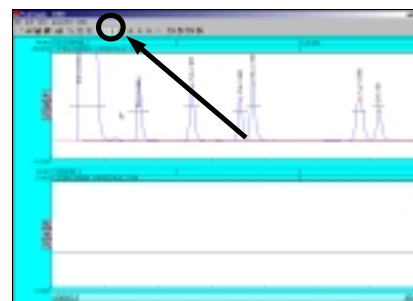
- After selecting OK from the Recalibration level menu the Calibration menu for Toluene will pop up. Check to make sure the flashing asterisk on the calibration curve is on level 3 and then click on the **Accept New** button to the right of the window.
- Once the new data is accepted, click on the **Method** button immediately below the Accept New button. The Recalibration type window will now open allowing the user to select a method of calibration. By default the calibration type is set at Multiple Line Segments. Select the **Quadratic (Ax<sup>2</sup>+Bx+C)** radio button and then click on **OK** with the mouse cursor.
- After changing the method of calibration click on **Statistics** in the upper right hand corner of the Calibration level window. The Calibration statistics window will pop up revealing the statistics for the calibration of Toluene. Click **OK** with the mouse cursor to close the Calibration statistics window and then select **Close** from the Calibration window to finish calibrating Toluene.



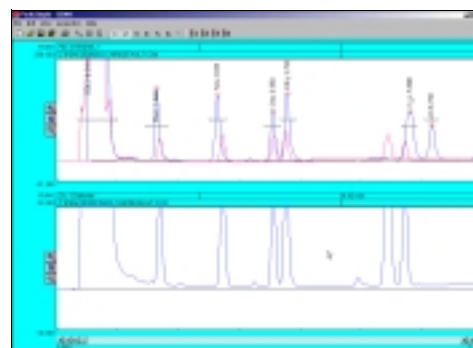
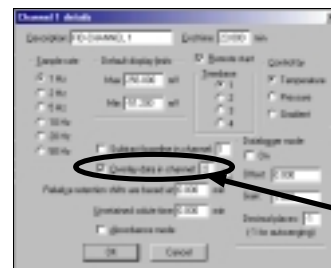
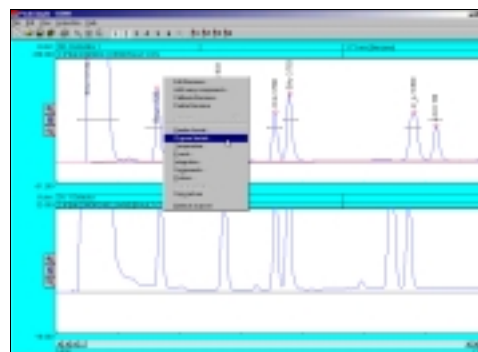
## Overlay

- To compare two or more chromatograms overlay them using PeakSimple. To overlay two chromatograms first open chromatogram 602.CHR and then click on the **2** button in the PeakSimple toolbar. A second chromatogram channel is now open in the PeakSimple window.
- Once the second channel is open select **File** from the PeakSimple menu bar and then click on **Open**. The Load chromatogram file window will open up displaying a list of files to load. Select chromatogram **FID602.CHR** to load and then select the **2** channel radio button to load the chromatogram in the second channel.

2

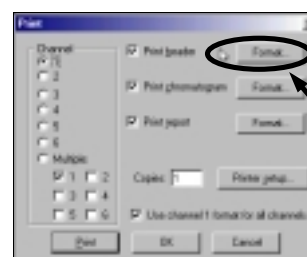
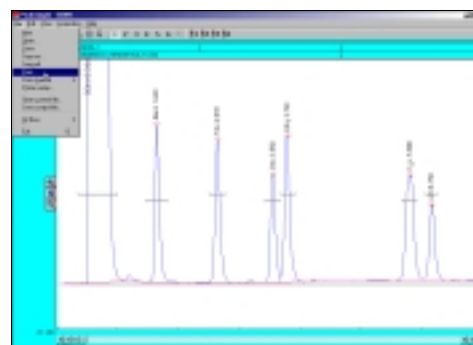


- Once FID602.CHR is open in the second channel right click using the mouse on the chromatogram in the first channel and select **Channel Details** from the list of options.
- After the Channel 1 details window appears on the screen locate the **Overlay data in channel** check box and select it. Look to the dialogue box to the right of the Overlay data in channel check box and insert the number **2** in place of the 1. Click on **OK** with the mouse cursor to exit the Channel 1 details window.
- The chromatogram FID602.CHR is now in place overlaid on top of chromatogram 602.CHR in channel 1. Chromatogram 602.CHR is in blue while FID602.CHR is in red.



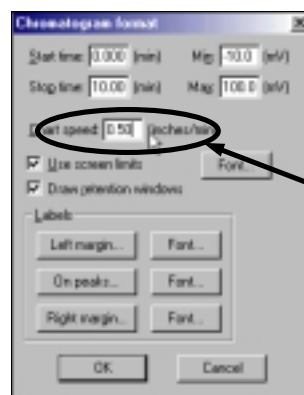
## Printing a Chromatogram

- To print a chromatogram first open chromatogram 602.CHR. Once the chromatogram is open select **File** from the PeakSimple menu bar and then select **Print** from the drop-down menu.
- The Print window will open and will allow the user to customize the printing of a chromatogram. Click on the **Format** button for the Print header to open up the Header format window. Add or delete any information in the window by clicking on the fields and inserting the desired information. Click on the **OK** button when all the desired information is inputted to close the window.

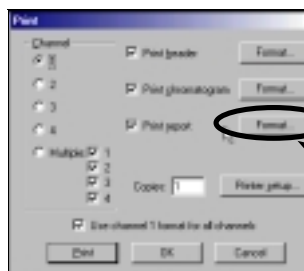




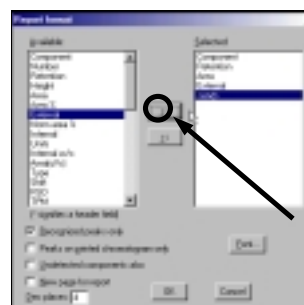
3. In the Print window click on the **Format** button for Print chromatogram to open up the Chromatogram format window. Locate the **Chart speed** dialogue box and insert the number of inches each minute on the chromatogram will take up when printed (for a nine minute run try **0.50** inches per minute). After the Chart speed is entered click on **OK** to exit the window.



4. In the Print window locate the Print report check box and click on the **Format** button to its right.



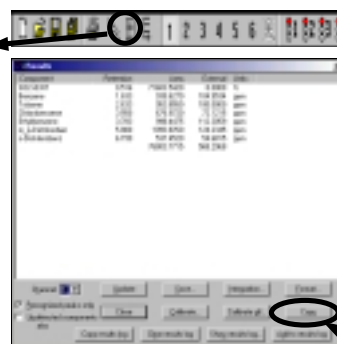
5. Once the Report format window is open click on **External** in the Available dialogue menu (on the left) and then click with the mouse cursor on the right facing arrow button to add External to the Selected dialogue box (on the right). After External is added to the Selected dialogue box click on **Units** with the mouse cursor and click on the right facing arrow button to add Units to the Selected dialogue box. Click on **OK** with the mouse cursor to exit out of the Report format window.



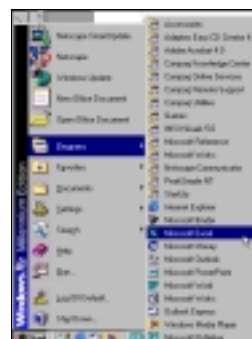
6. Select **Print** in the Print window to print the chromatogram or click on **OK** in the Print window to exit the window.

## Exporting to Excel

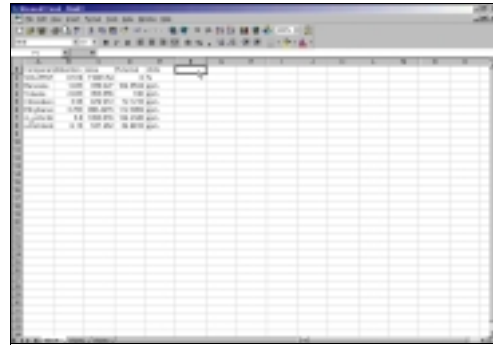
1. In the PeakSimple toolbar click on the **Results** window button to open up the Results window. Once the Results window is open click on the **Copy** button to copy the results data to the Windows clipboard.



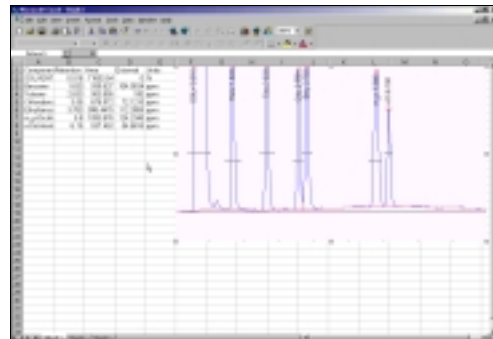
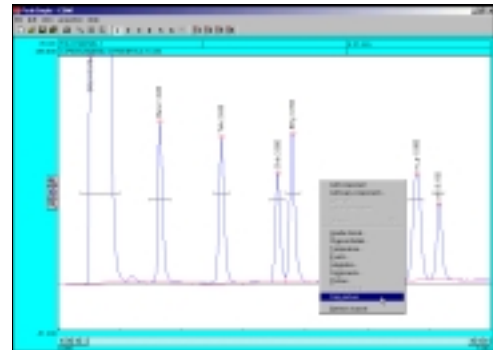
2. Make sure Microsoft Excel is loaded on the computer. If Excel is not loaded you can copy results data and chromatograms to Microsoft Word or PowerPoint. Open up Microsoft Excel by clicking with the mouse cursor on the **Start** button in the bottom left of the Windows screen and then **Programs** and then **Microsoft Excel** in the Windows Program menu.



6. Once Excel is opened select **Edit** from the Excel menu bar and then **Paste** from the drop down menu. The results data is now placed into the columns and rows of Excel. Using the mouse cursor, select a box to the right of the results data in the Excel spreadsheet. Go back into the PeakSimple for Windows NT program and hit **Close** to exit the Results window.



7. Right click with the mouse cursor anywhere on chromatogram 602.CHR and select **Copy picture** from the resulting menu. Go back into Excel and select **Edit** from the Excel menu bar and then **Paste** from the drop down menu. The PeakSimple chromatogram will now be displayed next to its results data in the rows and columns of Microsoft Excel.



This concludes the PeakSimple 2000 Basic Tutorial

