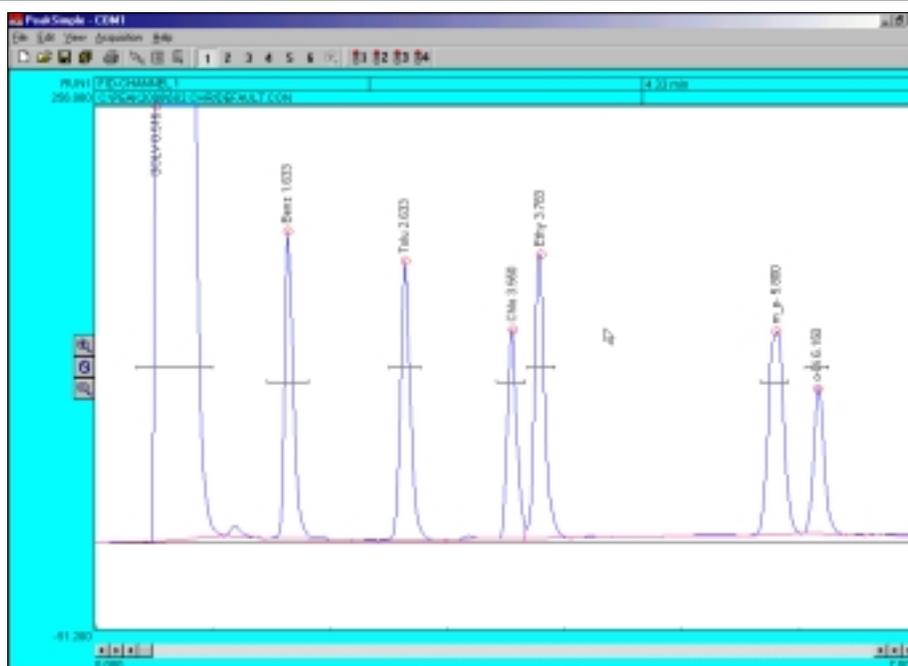


# PeakSimple 2000

## Chromatography Integration Software

### Advanced Tutorial



#### Installing PeakSimple 2000 from floppy disk or CD-Rom

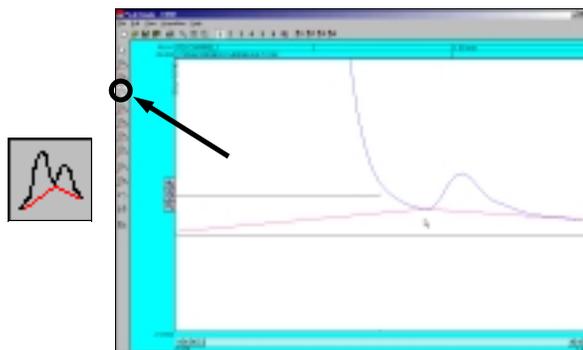
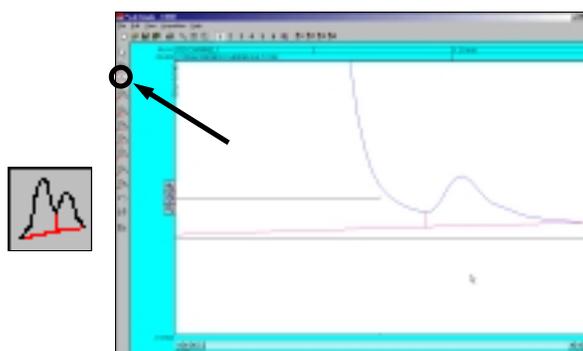
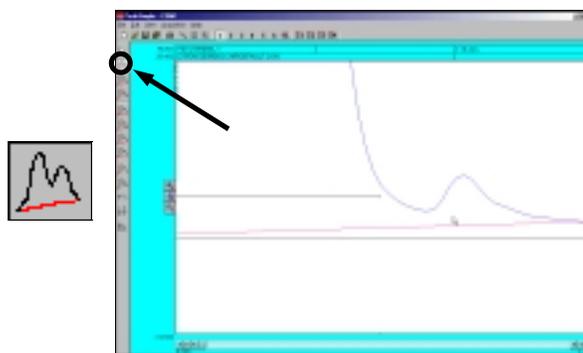
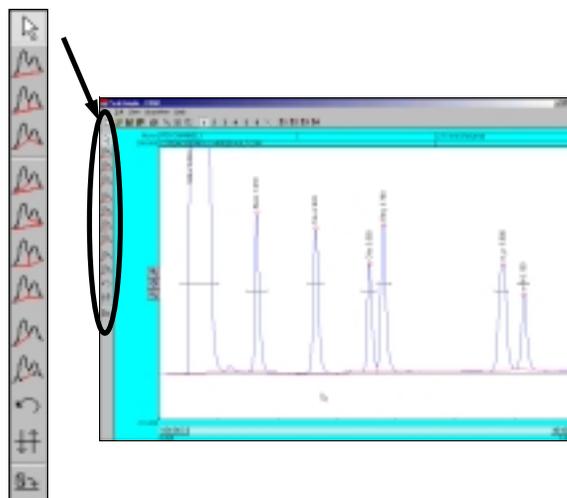
- Start the Windows operating system in use on your computer. (Windows 95, 98, ME, 2000)
- Insert the PeakSimple 2000 disk or CD into your disk drive.
- Go to the **Start** menu in the bottom left hand corner of the windows screen and select **Run** from the set of icons.
- From the run menu, type **X:\setup** (where **X** is the letter of your computers disk drive).
- Now click on the **Continue** button with your mouse cursor or press the enter key on your keyboard to begin installation.
- To complete installation follow the onscreen instructions during the installation wizard.

#### Installing PeakSimple 2000 from software download

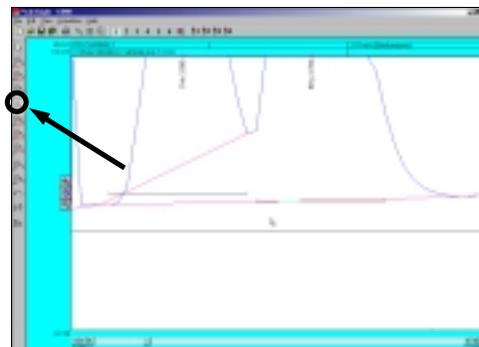
- Start the Windows operating system and use an online browser to access [www.srigc.com](http://www.srigc.com).
- From the menu on the left hand side of the screen select **Download our Software** and then download PeakSimple 2000 from the following page.
- Save the file to a temporary folder and then double click on it from My Computer to allow the program to self-extract.
- Once all the files have been extracted successfully double-click the install file and press the **Continue** button when prompted.
- Follow the onscreen instructions to complete the installation of PeakSimple.

## Manual Integration

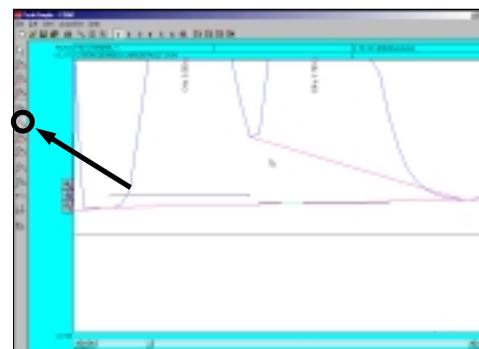
1. To manually integrate the PeakSimple baseline in a chromatogram use the manual integration tools found in the manual integration toolbar. To open the manual integration toolbar first have chromatogram 602.CHR loaded and then select **Edit** from the PeakSimple menu bar. From the drop down menu select **Manual integration** with the mouse cursor. The manual integration toolbar will now be displayed to the right of the PeakSimple toolbar in the left most part of the screen.
2. Use the None integration tool to add the area of the smaller peak to the area of the Solvent peak. First, zoom in on the solvent peak, the smaller peak to its right, and their baselines. Once the chromatogram is zoomed in select the **None** integration tool from the manual integration toolbar. With the None integration tool selected click once, using the left mouse button, on the valley between the solvent peak and the smaller peak.
3. Use the Drop integration tool to drop the baseline from the valley of the two peaks to an existing baseline. To drop the baseline select the **Drop** integration tool from the manual integration toolbar. Using the mouse cursor, click on the valley between the solvent peak and the smaller peak to drop the baseline.
4. The Based integration tool raises the baseline to the valley between two specified peaks. With the baseline dropped, click on the **Based** integration tool button and then click on the valley between the solvent peak and the smaller peak to raise the baseline to the valley.



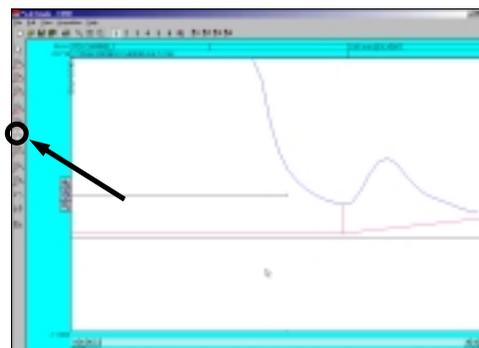
5. The Lead skim integration tool allows a peak's area to be skimmed off of the leading edge of another peak. To use the Lead skim tool first unzoom off of the solvent peak and the other smaller peak and then zoom in on the Chlorobenzene peak, the Ethylbenzene peak, and the baseline. After the chromatogram is zoomed click on the **Lead skim** integration tool button and then click on the valley between the two peaks with the mouse cursor.



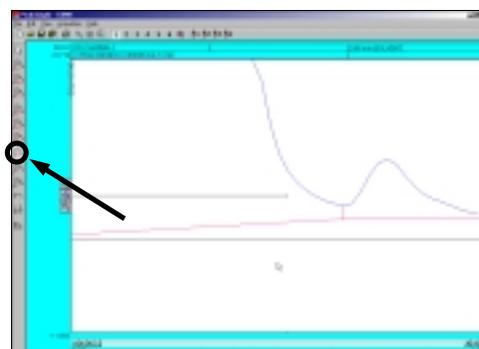
6. The Trail skim integration tool is similar to the Lead skim tool except a peak's area is now skimmed off of the trailing edge of another peak. Select the **Trail skim** tool button from the manual integration toolbar and then click on the valley between the Chlorobenzene and Ethylbenzene peaks with the mouse cursor to see the Ethylbenzene peak skimmed off of the Chlorobenzene peak.



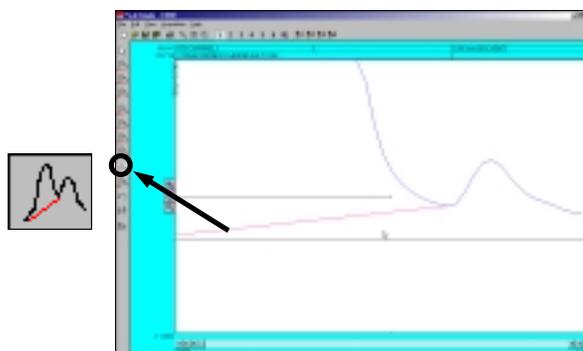
7. The Lead horizontal tool constructs the baseline horizontally for the leading peak while the trailing peak's baseline stretches from the horizontal line to the next valley. Unzoom off of the Chlorobenzene and Ethylbenzene peaks and instead zoom in on the Solvent peak, the smaller peak to its right, and the baseline. Click on the **Lead horizontal** integration tool in the manual integration toolbar and then click, using the left mouse button, on the valley between the solvent peak and the other smaller peak.



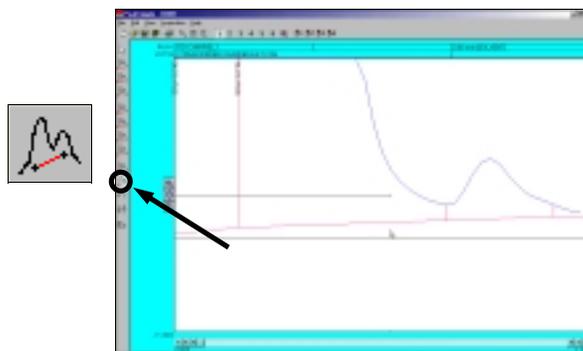
8. The Trail horizontal integration tool drops the baseline horizontally for the trailing peak while the lead peak's baseline stretches from the horizontal line to the previous valley in the chromatogram. After selecting the **Trail horizontal** tool in the manual integration toolbar click with the mouse cursor on the valley between the two zoomed in peaks.



9. The Inhibit tool ends the baseline after a valley effectively inhibiting a peak's area from being counted with the rest of the chromatogram. To use the Inhibit integration tool select the **Inhibit** tool button from the manual integration toolbar and click on the valley of the Solvent peak and the smaller peak to its right.



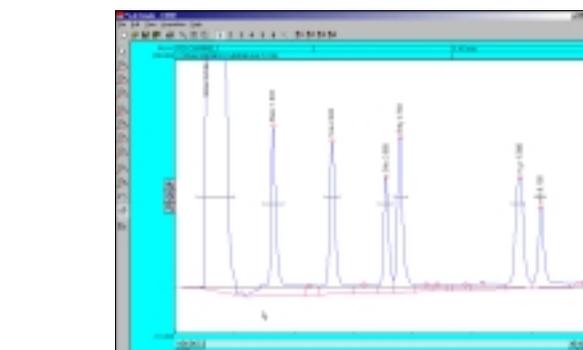
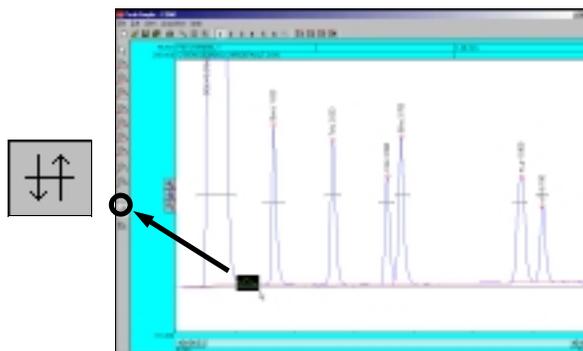
10. The Rubber Band tool is used to manually draw the baseline in a chromatogram. To use the Rubber Band tool first scroll the X-axis scrollbar all the way to the left to **0.000**. Select the **Rubber Band** tool from the manual integration toolbar and draw a line from the valley between the Solvent peak and the small peak to its left to the valley between the smaller peak to the right of the Solvent peak and the peak to its right.



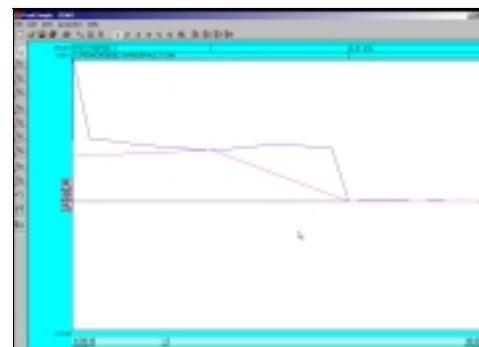
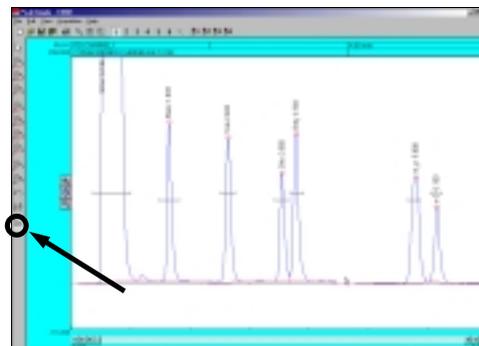
11. To undo a change made to the baseline of a chromatogram with the manual integration tools use the Undo button found in the manual integration toolbar. To undo the changes made to the baseline using the Rubber band tool click on the **Undo** button with your mouse cursor. All changes made to the baseline will now be undone.



12. The Reverse tool allows the inverting of a peak in a chromatogram. **Note:** To reverse the orientation of the X-axis in real time go to the Events table. First unzoom off of the Solvent peak and the smaller peak to its right and then select the **Reverse** tool from the manual integration toolbar and click and hold the left mouse button while the area of the chromatogram you want to reverse is dragged over with a black box. Let go of the mouse button when the desired area is selected to reverse the orientation.

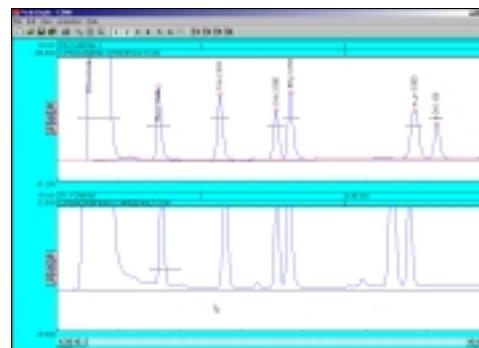


13. The Zero tool is used to set the value of the data line at a selected point and following in the chromatogram to zero. First undo the changes done to the chromatogram by the Reverse tool by reopening 602.CHR in the PeakSimple menu bar. **Note:** Changes made to a chromatogram by the Reverse tool and the Zero tool cannot be undone with the Undo tool. Once the file is reopened click on the **Zero** tool and click anywhere on the baseline between the Ethylbenzene peak and the two peaks to its right with the mouse cursor to set the data line at zero.



## Creating Component Tables

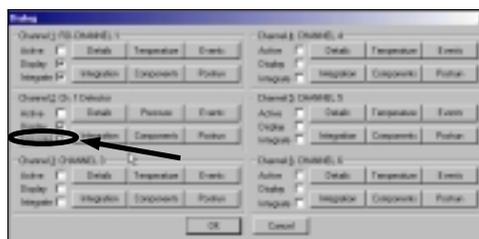
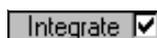
1. To create a component table from scratch open up a second channel in the PeakSimple window by clicking on the Display Channel 2 button in the PeakSimple toolbar. Once the second channel is open click on **File** and then **Open** to get to the Load chromatogram file window. Select file **FID602.CHR** from the list of files and select the Channel 2 radio button to open the file in channel 2. Click **OK** with the mouse cursor to load the file.
2. In channel 2 locate the second tall peak from the left and right click on it with the mouse cursor. From the resulting menu select **Add component** to add a retention window bar to the peak. Once again right click on the peak and select **Edit component** from the menu to open up the Component details window.



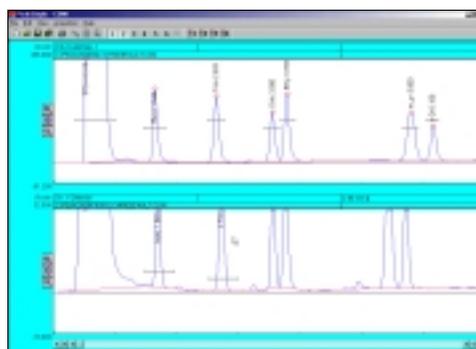
- Once the Component details window is open locate the Peak number dialogue box and add the number **1**. Immediately underneath the Peak number box is the Peak name dialogue box. In the Peak name dialogue box input **benzene** to name it. Locate the Units box and put **ppm** to make the units parts per million. Locate the In case of multiple peaks options box and select the radio button for **Show largest peak only**. Click on **OK** with the mouse cursor to close the window.



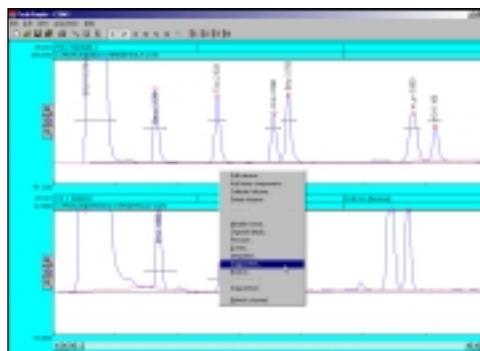
- Go to **Edit** in the PeakSimple menu bar and then **Channels** from the resulting menu. The Channel controls window is now open. Locate the Channel 2 options box and the Integrate checkbox. Check the **Integrate** checkbox and then click on **OK** with the mouse cursor to close the window. The peak in the second channel should now identify itself as benzene.



- Locate the large peak to the right of the benzene peak in the second channel. Right click and then select **Add component** to add a retention window bar to the peak. Right click again and go to **Edit component** to open up the Component details window. Change the Peak number to **2**, the Peak name to **toluene**, the Units to **ppm**, and the In case of multiple peaks options box to **Show largest peak only**. Click on **OK** with the mouse cursor to exit the window.



- Right click anywhere on the second channel and select **Components** from the list of options. Once the Channel 2 components window is open make sure all the data is correct and then click on **Save** to save the Component data to disk. Name the file **Ctable** and then click on **OK** to close the window. An unlimited number of component windows may be added to the component table.



Channel 2 components

Peak	Name	Start	End	Calibration
1	benzene	1.000	1.100	
2	toluene	2.000	2.100	

Buttons: Add, Change, Remove, Calibrate, Load, Save, Use, Exit, OK

## Temperature Programming

- To modify the temperature programming in PeakSimple first open chromatogram 602.CHR and then right click anywhere on the chromatogram. From the drop down menu select **Temperature** to open up the Temperature control window.
- In the Temperature control window click using the mouse cursor on the set of numbers in the box and select **Change** from the group of buttons below. The Temperature segment details window will open allowing the modification of the temperature programming. Locate the Hold for dialogue box and insert a **2** in the box. Click on **OK** to close the window and go back into the Temperature control window.



Temperature segment details

Initial temperature  deg

Hold for  min

Then ramp at  deg/min

Until temperature is  deg  
(or for  min)

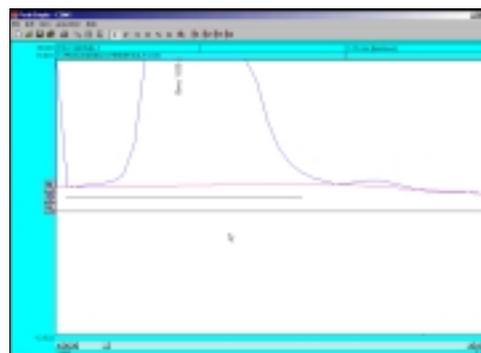
Buttons: OK, Cancel



- In the Event details window locate and select the relay **G** radio button with the mouse cursor and then locate the Event time dialogue box and enter **.1** in the box. Click on **OK** to exit the window. **Note:** *The relay might be used to actuate a valve when hardware is connected.* The event type will now be added to the Events table. Select the **Add** button and now locate and select the **Zero** event type radio button. Leave the Event time box at 0.000 and once again click on **OK** to exit the window and add the event to the Events table. **Note:** *The Zero event auto-zeros the detector signal at the beginning of the run.* Click on the **Add** button again and select the **Integration-Based immediate** radio button in the Event details window and input **1.86** in the Event time dialogue box. Select **OK** to exit the window.

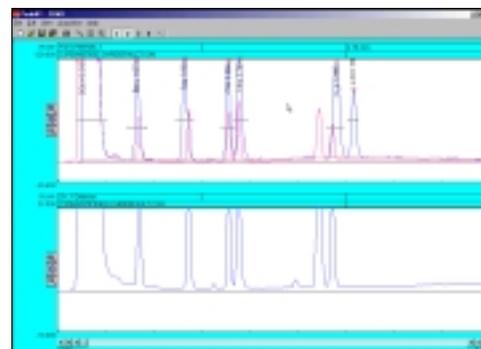
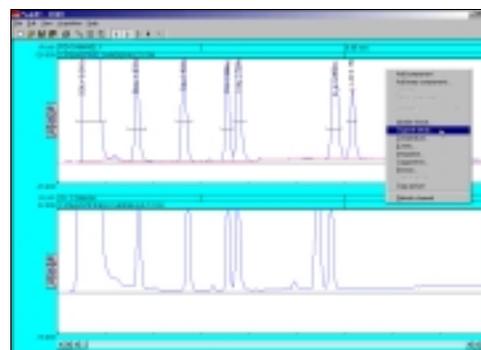


- There are now three events in the Events table. Click on **OK** to exit the Events window and then hit the **Enter** button on the keyboard to reintegrate the baseline according to the events in the Events table. Notice that the baseline is connected to the data line at 1.86 minutes.

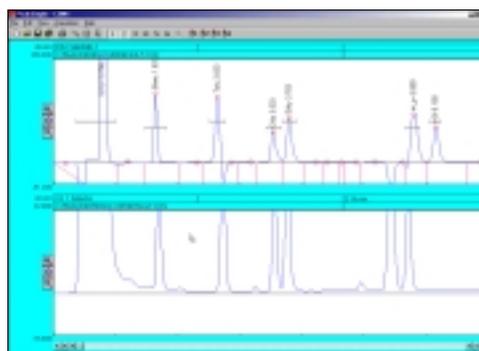
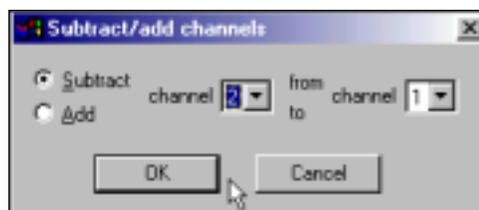
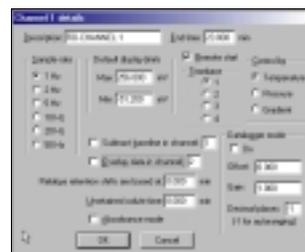
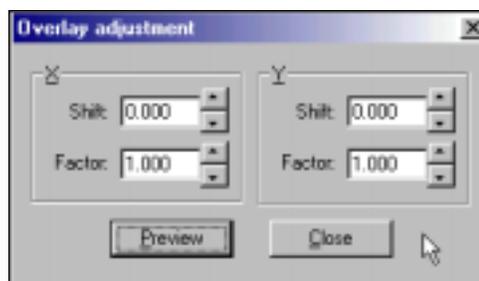


## Overlay and Subtract

- To overlay one PeakSimple chromatogram on top of another chromatogram open up a second channel in the main screen and load chromatogram 602.CHR in the first channel and chromatogram FID602.CHR in the second channel. Right click anywhere in the first channel and select **Channel details** from the drop down menu.
- In the Channel 1 details window locate the Overlay data in channel checkbox and check it and then input a **2** in the dialogue box to the right. The chromatogram in channel 2 is now overlaid on top of the chromatogram in channel 1. The overlay appears in a different color.



- Right click anywhere on the first channel and select **Overlay adjustment** from the drop down menu. In the Overlay adjustment window locate the Factor scroll box in the X box. Experiment scrolling the X factor up or down to shift the overlaid chromatogram to its right or left. Locate the Factor scroll box in the Y box and experiment scrolling the Y factor up or down to move the overlaid chromatogram up or down. Click on the **Close** button to close the window.
- To subtract a chromatogram in one channel from another channel, right click using the mouse cursor on channel 1 and select **Channel details**. From the Channel 1 details window deselect the Overlay data in channel checkbox and then click on the **OK** button to exit the window.
- Go to the **Edit** menu bar and select **Subtract/Add channels** from the drop down menu. In the Subtract/add channels window make sure the Subtract radio button is selected and that channel 2 is being taken from channel 1. Click on the **OK** button to make the changes take effect and have channel 2 subtracted from channel 1. The normal way to use this feature is to subtract a drifting baseline from a chromatogram.

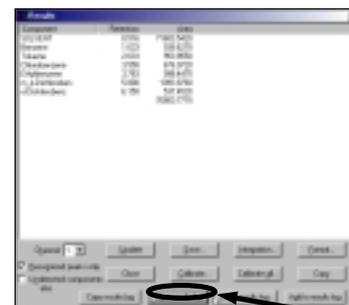


## Results Log

- Open chromatogram 602.CHR in the PeakSimple main screen and then select the **Results** button from the PeakSimple toolbar. In the Results window click on the **Clear results log** button at the bottom of the window. Click on **Yes** from the resulting window to clear the results.
- Locate the **Add to results log** button and click on it three times to add the results on the screen to the Results log three times. Click on the **Show results log** button to view the results log in the Windows Notepad. Exit the Windows Notepad program by selecting **File** from the menu bar and then **Exit**.



Clear results log



- In the Results window locate the **Copy results log** button at the bottom of the window and click on it with the mouse cursor (don't confuse the Copy button with the Copy results log button). Open up Microsoft Excel (or if Excel is not loaded Microsoft Word or PowerPoint) and select **Edit** from the menu bar and then **Paste** to copy the results log to Excel.
- Go back into PeakSimple and close the Results window by selecting the **Close** button. Right click using the mouse cursor on the chromatogram and select **Postrun** from the drop down menu to open the Post-run actions window. From the window locate the Add to results log checkbox and add a check to the box. By selecting the Add to results log checkbox all results from data analysis will automatically be added to the results log after the run is done. Click on **OK** to exit the window. In this way a summary of many analyses can be automatically created and then exported from PeakSimple.



This concludes the PeakSimple 2000 Advanced Tutorial

Further documentation can be obtained by going to:  
[www.srigc.com](http://www.srigc.com) online

If you have questions or would like to place an order call:  
 (03) 9762 2034 in Australia