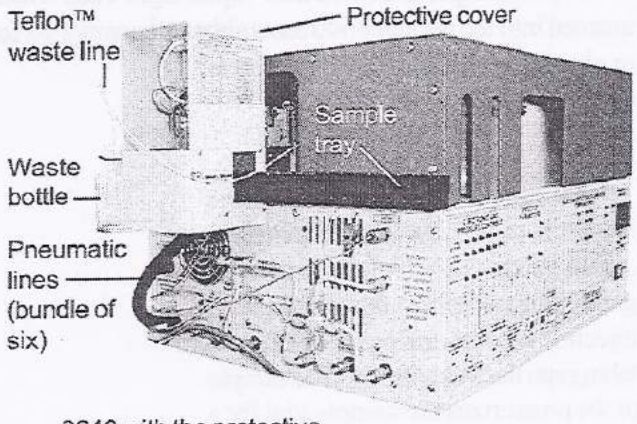
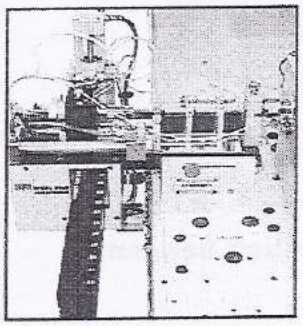
Overview

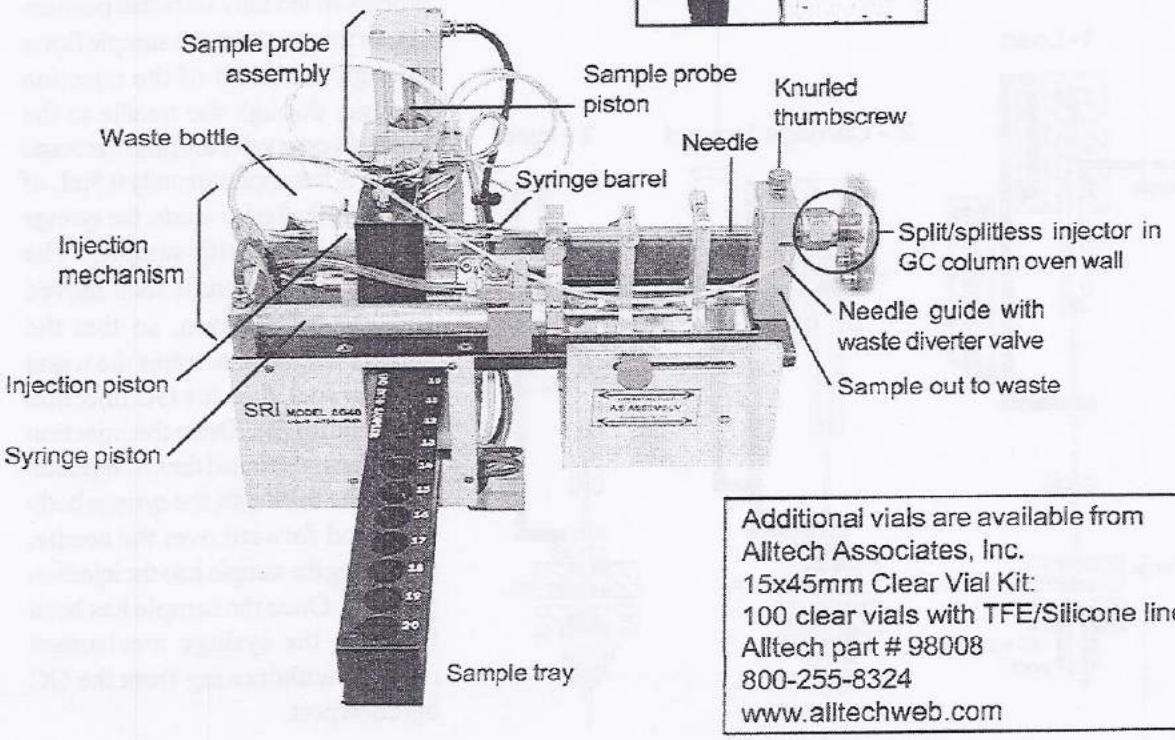
The SRI Model 8640 20-vial liquid autosampler is installed on the left-hand side of the SRI 8610C GC. The 8640 connects to an additional injector on the left side of the column oven. This additional injector may be on-column, heated, or split/splitless. It uses a sample tray to hold up to twenty 2mL vials, a sample probe to transfer the sample from the vials into the syringe barrel, and an injection mechanism to deliver the sample from the syringe barrel, through the needle, into the injector in the GC column oven wall. The 8640 uses 60psi of air or nitrogen to actuate its moving parts. The 8640 functions are assigned relays so that the autosampler may be operated automatically using a PeakSimple event table.

The 8640 is shipped with 100 screw-top vials and septa, replacements for which are available from a variety of suppliers. Extra sample trays and cooled sample trays are available. The cooled sample trays require an external refrigerated lab circulator.



8640 with the protective cover removed





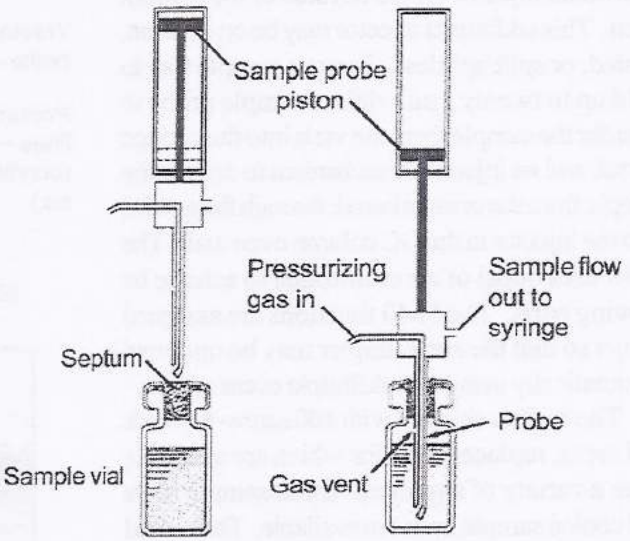
Additional vials are available from
Alltech Associates, Inc.
15x45mm Clear Vial Kit:
100 clear vials with TFE/Silicone liners
Alltech part # 98008
800-255-8324
www.alltechweb.com

Theory of Operation

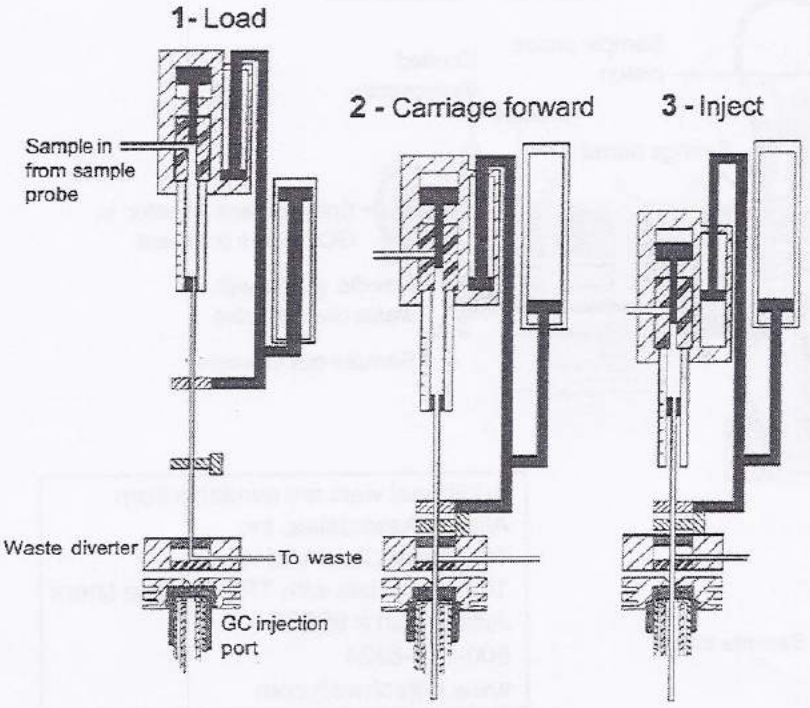
Liquid sample is sealed into vapor-tight vials which are inserted into the sample tray. The tray is then inserted into the Model 8640 assembly and positioned for the sampling sequence. The 8640 uses 60psi of air or nitrogen to actuate its moving parts.

The sampling probe, a concentric needle, is moved down by a piston to pressurize the vial with helium or other gas, causing sample to flow through the injection syringe and out the Teflon™ tubing into the waste bottle. The sample probe pressurizes the sample vial for a period of time long enough to rinse the previous sample to waste and fill the syringe with sample.

Sampling Probe Sequence



Injection Sequence

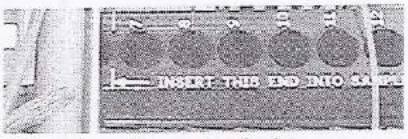


The syringe mechanism begins the process in the fully retracted position (1). In this position, the sample flows through the barrel of the injection syringe, through the needle to the waste diverter valve and into the waste bottle. After approximately 0.5mL of sample is flushed to waste, the syringe barrel is filled with sample. The syringe mechanism is then moved forward by a piston, so that the syringe needle penetrates the waste diverter seal, then the GC injection port septum (2). Once the injection needle has penetrated the GC injection port to the full depth, the syringe body is pushed forward over the needle, displacing the sample into the injection port (3). Once the sample has been injected, the syringe mechanism retracts, withdrawing from the GC injection port.

General Operating Procedures

1. Fill each 2mL vial at least 75% full with liquid sample. Close the vials so that they are vapor-tight, with the Teflon side of the vial septa facing downward into the vial.

2. The sample tray is inserted and removed from the 8640 in one direction only. To remove the sample vial tray, push it away from you, toward the back of the GC, until it is free of the autosampler assembly. Place the filled sample vials in the tray. Reinsert the sample tray into the 8640 assembly from the front. Push it gently toward the back of the GC until the white lines at the tip of the white arrow on the sample tray are aligned with the front edge of the 8640. The sample tray is then in the ready position, with vial number one in place under the sample probe. The sample tray shown below, right is almost in the ready position (it was left partially out for visibility of the lines and arrow).



3. Activate and heat the GC detector(s).

4. Load or create a column oven temperature program.

5. Load or create an event table. Version 2.74 (and higher) of the PeakSimple software includes an event table file called "8640as.evt" as a general event table for use with the 8640 autosampler. When you load this event file, the default relay descriptions will not match the actual 8640 autosampler relay descriptions. These autosampler-specific descriptions must be entered by you, the user. The relays assigned to the autosampler are as follows:

Relay A - moves the sample probe DOWN
Relay B - moves the sample probe UP.
Relay C - moves the syringe carriage FORWARD
Relay D - INJECTS the contents of the syringe
Relay E - ADVANCES the tray one position
Relay F - PRESSURIZES the sample vial

WARNING!
To avoid injury, keep your hands clear of the 8640 during operation.

See the event table shown at right for appropriate descriptions. The 8640 relay descriptions are also labeled on the right-hand side of the GC.

8640.evt		
EVENT TIME	EVENT	EVENT FUNCTION
0.000	ZERO	Zero data system signal
0.050	A ON	Sample probe DOWN
0.100	F ON	Vial pressure ON (pressurize the sample vial)
0.650	A OFF	Release pressure holding sample probe DOWN
0.700	F OFF	Vial pressure OFF
0.750	B ON	Sample probe UP
0.800	C ON	Syringe carriage FORWARD
0.850	D ON	Sample syringe INJECT
1.000	C OFF	Syringe carriage RETRACT
1.050	D OFF	Sample syringe RETURN
1.100	E ON	Tray advance ON
1.200	E OFF	Tray advance OFF
1.300	B OFF	Release pressure holding sample probe UP

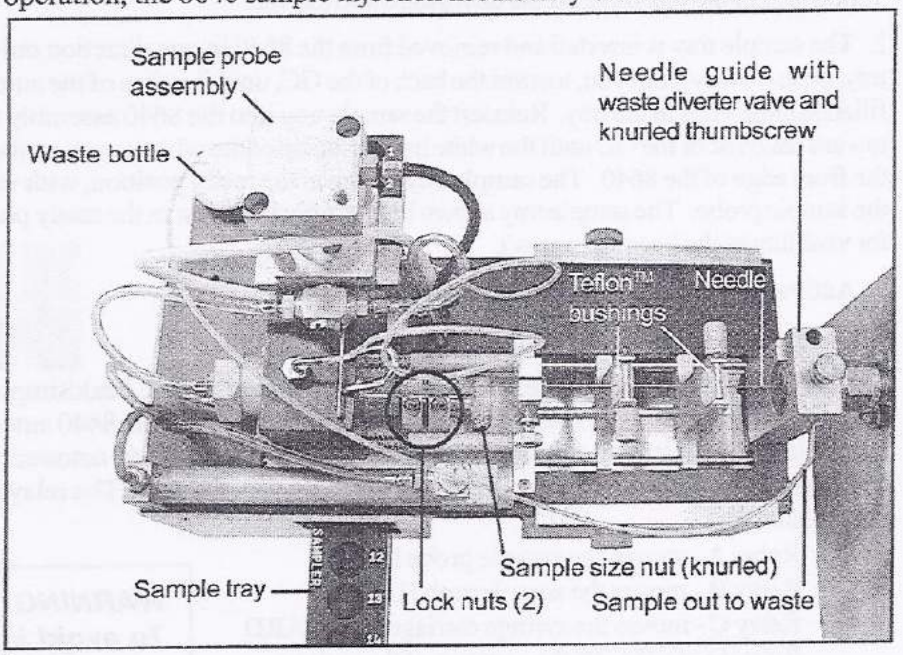
6. Set the autosampler air or nitrogen tank to 60psi. Set the carrier gas to 10mL/minute (the equivalent psi setting for your machine is labeled on the right panel of the GC). The amount of sample used to flush the needle can be adjusted by varying the pressure of the gas used to force the sample from the vial. This gas pressure is adjusted with the EPC trimpot on the top edge of the GC's front control panel, located directly above the vertical label "VIAL PRESSURE" on the front control panel. Using the event table at right, you should count 25 drops during the time that the gas is pressurizing the sample (0.600 minutes).

7. The injection volume is factory set at 1µL, but is adjustable to 0-3µL. Loosen the 2 hex-head lock nuts, then turn the knurled nut while observing the needle in the syringe barrel to achieve the desired injection volume (please see the picture on the ***Changing the Needle*** page to locate the lock nuts and knurled nut).

Changing the Needle

In the course of normal operation, the 8640 sample injection needle may become bent or otherwise damaged and require replacing. Make sure the syringe mechanism is fully retracted before starting; this is the default position to which it should return after a sample injection sequence.

Replacement needles are available from Central Instruments under part number 502743. Syringe barrel and needle sets are available under part number 503188. Call Central Instruments at:
225-261-1917
Or write to:
P.O. Box 337
Greenwell Springs, LA 70739
USA.



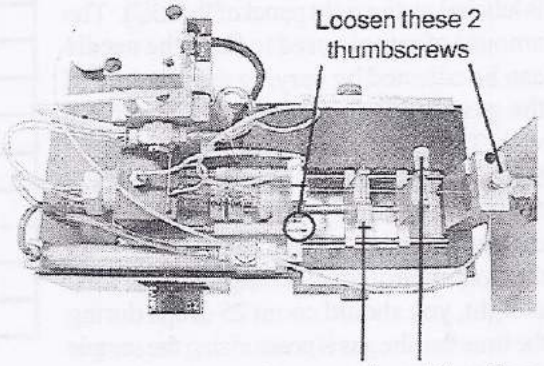
1. To remove the needle, loosen the thumbscrew on the top of the waste diverter and the thumbscrew on the needle guide closest to the syringe barrel. Loosen and remove the two bushing retainers. Carefully lift out the needle, the two Teflon™ bushings and the waste diverter valve together. You will have to push the waste diverter valve out of the needle guide, and angle the needle tip out through the slot in the side of the waste diverter needle guide as you pull the needle from the syringe barrel.

2. Slide the waste diverter valve and the two Teflon™ bushings off the old needle and onto the replacement needle.

3. Place the needle into the thumbscrew needle guide and the syringe barrel, and carefully angle the needle with the bushings and waste diverter valve into place, using the slot in the waste diverter needle guide to get the tip of the needle into alignment with the syringe barrel.

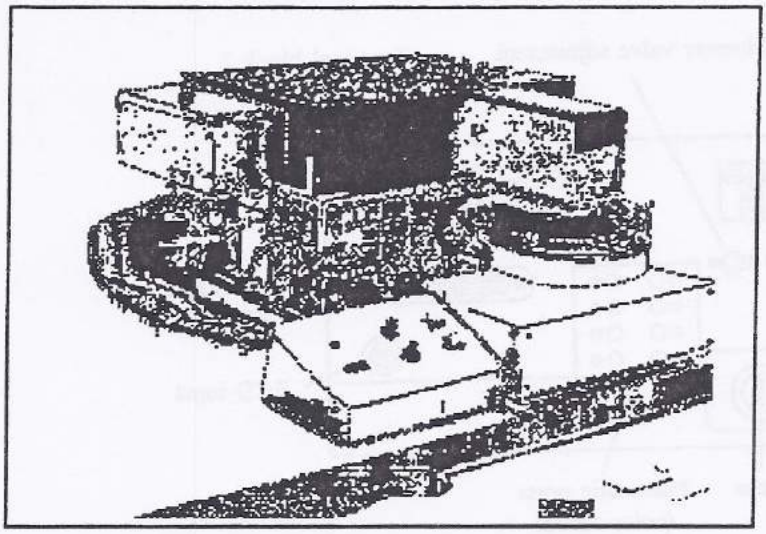
4. Position the two bushings in their cradles, then replace and tighten the bushing retainers. Tighten the thumbscrews on the needle guide and waste diverter.

5. Adjust the sample injection volume by loosening both hex-head lock nuts, then turning the knurled thumbscrew to achieve the desired volume. Tighten the lock nuts.



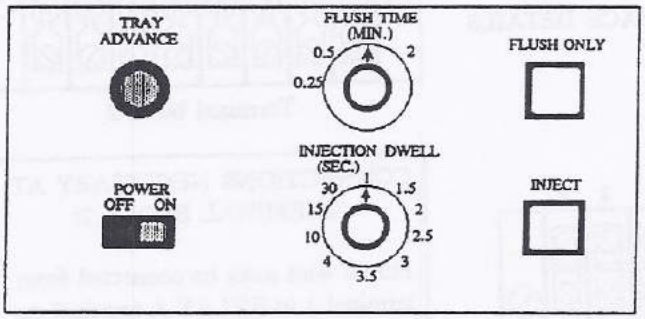
Chapter: INSTALLATION

Topic: Interfacing The Liquid Autosampling Carousel



SRI liquid autosampler connected to SRI 8610 gas chromatograph

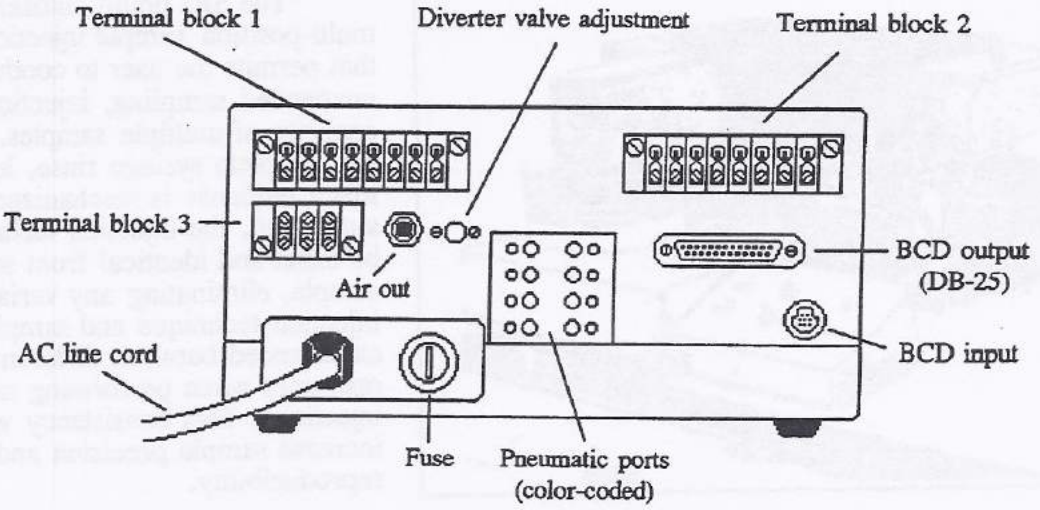
The SRI liquid autosampler is a multi-position sample injection system that permits the user to conduct unattended sampling, injection and analyses of multiple samples. Because the complete syringe rinse, load and inject sequence is mechanized and automated, the injection technique will be exact and identical from sample to sample, eliminating any variation in injection technique and sample delivery experienced between different operators when performing manual injections. This consistency will increase sample precision and reproducibility.



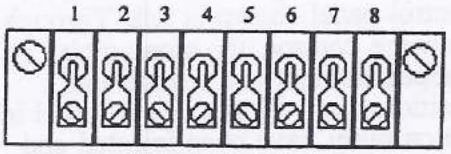
Front control panel of SRI autosampler controller

The autosampler is controlled automatically by PeakSimple software and/or manually at the autosampler control panel shown at left. Through software control, the autosampler is stepped through the sample vial positions until all samples inserted in the carousel have been injected and analyzed (without the need for operator intervention). A simple command in the event table (momentary activation of relay A) causes the autosampler to insert, flush, draw and inject the needle contents into the injection port. As soon as the needle has been withdrawn from the injection port, the autosampler is stepped to the next vial position to remain at the ready for the next actuation of relay A.

The sample vial tray may be manually advanced by hand or by pressing the TRAY ADVANCE actuator button. The amount of time (in minutes) that the syringe needle is flushed to clear the preceding sample is selectable using the FLUSH TIME control. The amount of solvent used to flush the syringe may also be varied by adjusting the sample pressurizing gas pressure. The actual volume of flush required will be dictated by the characteristics of the sample being injected. If not overly viscous, a sample flush volume of approximately 100 microliters should be adequate. If sample availability is limited to small volumes, then the flush may need to be reduced to economize on sample consumption. The amount of time that the needle remains in the injection port after the sample has been discharged from the syringe is also selctable using the INJECTION DWELL control. Selectable in seconds, the control permits the user to choose having the needle withdraw immediately upon having deposited its sample, or to maintain the needle in the injection port for an extended period, permitting any sample containing higher boiling or thermally labile components adequate time to exit the syringe and enter the injection port. High boiling components require longer needle-injection port dwell times than volatile components. A setting of 1 second signifies that the needle penetrates the septum, injects the sample and is withdrawn immediately, all within the duration of one second. A setting of 4 seconds permits the needle to dwell in the injection port for an additional 3.5 seconds.

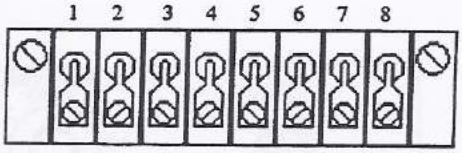


View of rear panel of SRI autosampler controller unit



Terminal block 1

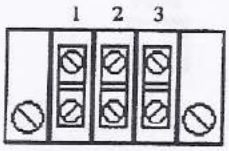
REAR PANEL INTERFACE DETAILS



Terminal block 2

CONNECTIONS NECESSARY AT TERMINAL BLOCK 1:

A jumper wire must be connected between terminals 7 and 8 of this terminal block (index enable position). Black wire provided.



Terminal block 3

CONNECTIONS NECESSARY AT TERMINAL BLOCK 2:

Purple wire must be connected from terminal 1 to RELAY A terminal on interface board. Black wire must be connected from terminal 2 to D.GND terminal on interface board.

CONNECTIONS NECESSARY AT TERMINAL BLOCK 3:

Three-wire control cable from autosampler connects here. Black wire connects to terminal 1, red wire to terminal 2 and green wire to terminal 3

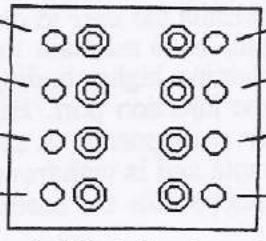
PNEUMATIC HOSE TERMINAL

White hose from autosampler

Green hose from autosampler

Red hose from autosampler

White hose from autosampler vial pressurization regulator



Clear hose from autosampler

Black hose from autosampler

Yellow hose from autosampler

Blue hose from tray rotation pneumatic pressure regulator

Terminal block is color-coded to match hose colors

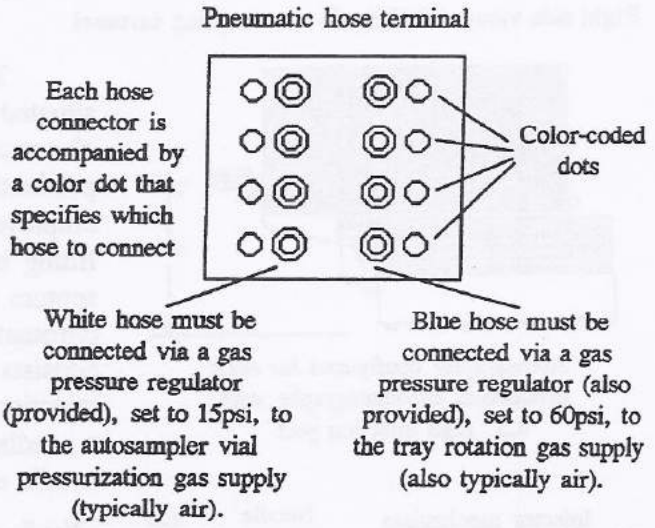
Chapter: INSTALLATION

Topic: Interfacing The Liquid Autosampling Carousel

The procedure for installation of the autosampling carousel is simple and straight-forward. Pneumatic and electrical connections must be made at the controller unit and at the data system interface board (if in use by the system). Once these connections have been made, the autosampler is inspected for proper docking height with the chromatograph injection port. If the autosampler is intended for use with an early version of the model 8610 chromatograph (low-profile chassis with an injection port 6.5" above the countertop), the carousel will be equipped with three rubber feet that elevate the injection needle axis to exactly 6.5". Current production models are mounted on a platform that elevates the injection needle axis to exactly 10". This corresponds to the injection port height of the current production model 8610 chromatograph. When proper unit height has been verified at the injection port, the autosampler is mated to the chromatograph and operation may begin.

PNEUMATIC CONNECTIONS

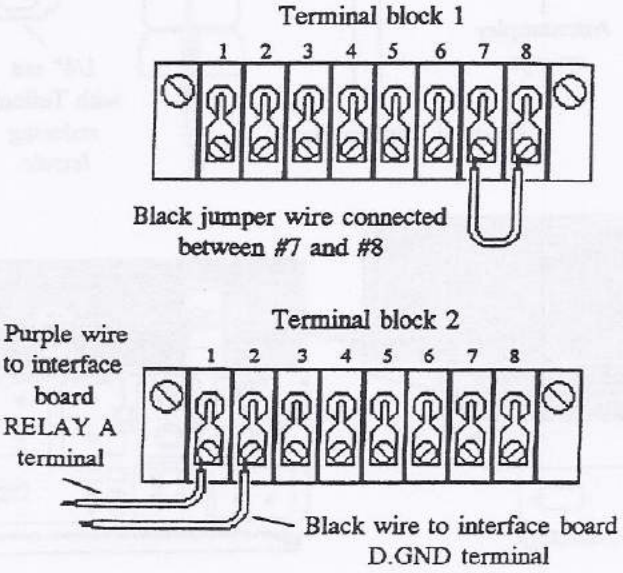
In addition to connecting the six color-coded hoses from the autosampler control harness to their respective pneumatic terminals on the rear of the autosampler controller unit, two gas connections must be made at the lower two pneumatic hose terminals on the bulkhead. The white hose provided must be connected to the autosampler vial pressurization gas supply, using the provided regulator. This regulator should be set to 15 psi. Gas (typically air or nitrogen) is injected into the vial by the outer sleeve of the concentric sampling needle (needle within a needle), forcing sample to flow out of the vial through the center needle and into the injection syringe. The blue hose should be connected to the tray rotation gas supply, set to 60psi with the other regulator provided with the unit. This gas enables the tray mechanism to rotate, advance the samples and operate the injection mechanism.



If air is used by both regulators, the main air supply pressure should be regulated to (at least) 75psi in order to maintain a stable gas supply.

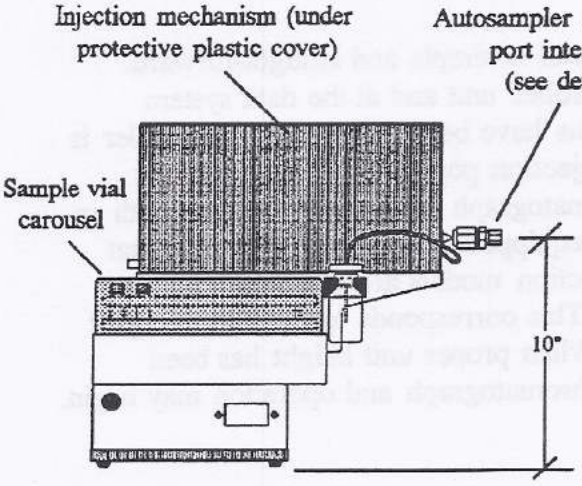
ELECTRICAL CONNECTIONS

There are only three connections to be made by the user. A black jumper wire (provided) must be connected between terminals 7 and 8 of terminal block 1. The purple and black wires (also provided) must be connected to the interface board terminals labeled RELAY A and D.GND, respectively. These two wires provide the remote activation of the autosampler advance and sample circuitry (same as INJECT on the controller unit) by the data system or other remote device.



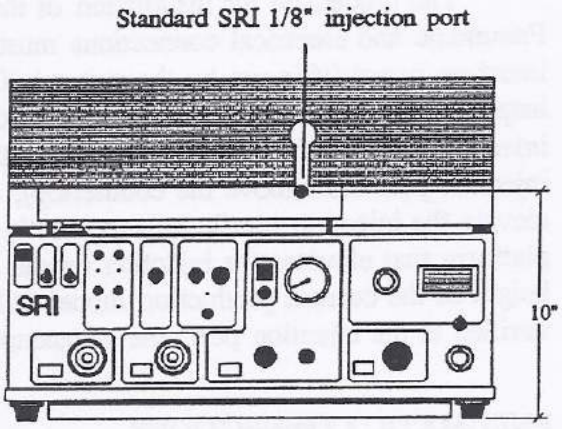
Chapter: INSTALLATION

Topic: Connecting The Autosampler To The Chromatograph Injection Port

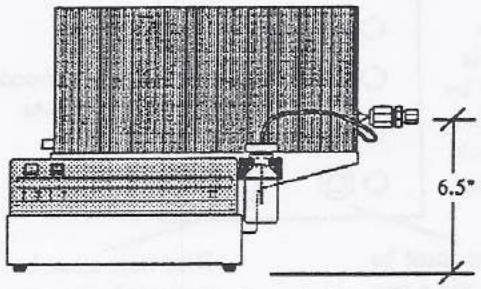


Right side view of SRI liquid autosampling carousel

Autosampler injector extends from injection mechanism (under cover) at a height of 10" from the countertop, equal to the SRI chromatograph injection port height

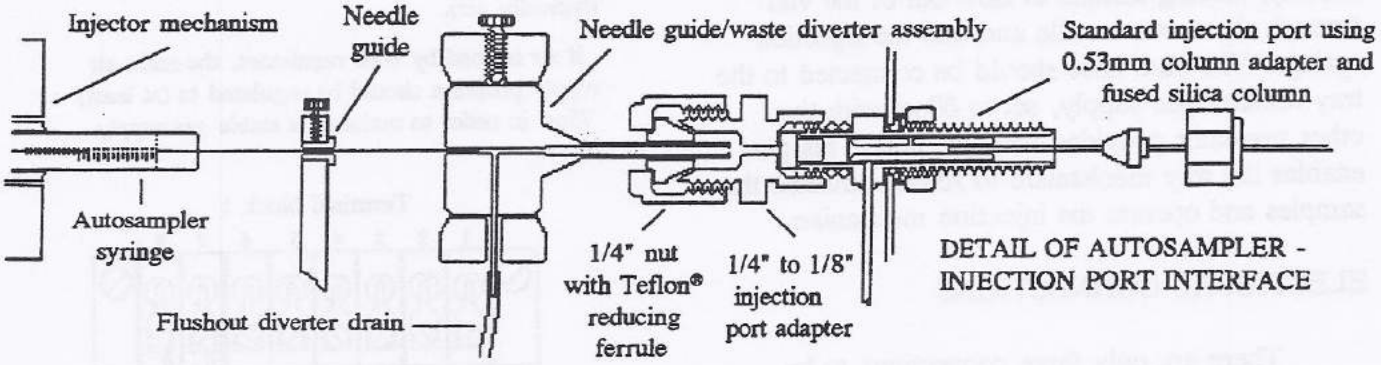


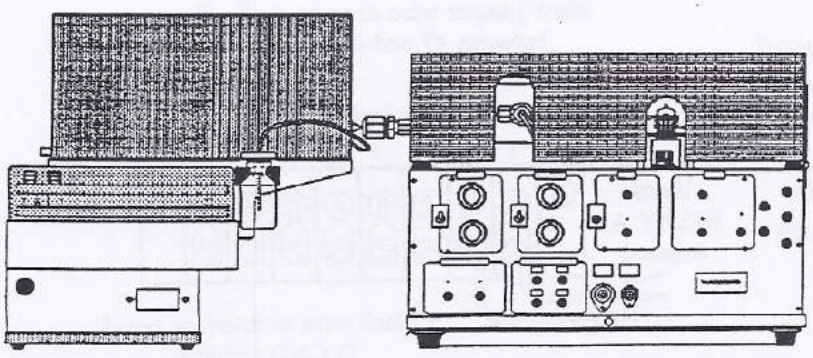
Front view of SRI model 8610 gas chromatograph



Autosampler configured for early production chromatographs with 6.5" high injection port

The SRI liquid autosampler injector mechanism is situated at a height equal to the injection port of the chromatograph. The injection port height of current production units is 10" (25.4cm). Previous models (pre-1992) employed an injector height of 6.5" (16.5cm). A special fitting is supplied with the autosampler that replaces the septum nut normally used to seal the injection port of the chromatograph. This fitting, also containing a septum, consists of a 1/8" to 1/4" adapter that is connected to the injection port. A special cylindrical brass fitting, employed as a needle guide and waste solvent diverter, is inserted into the needle end of the injector mechanism frame and secured by a thumbscrew. From this cylindrical fitting, a 1/8" metal tube protrudes. This tube, an extension of the needle guide, is secured to the chromatograph's injection port adapter by means of a 1/4" nut with a 1/4" to 1/8" Teflon® reducing ferrule. Once both fittings are in place, the units are docked together and the 1/4" nut is secured. Then the autosampler controller unit is located in a convenient location and normal operation can begin.



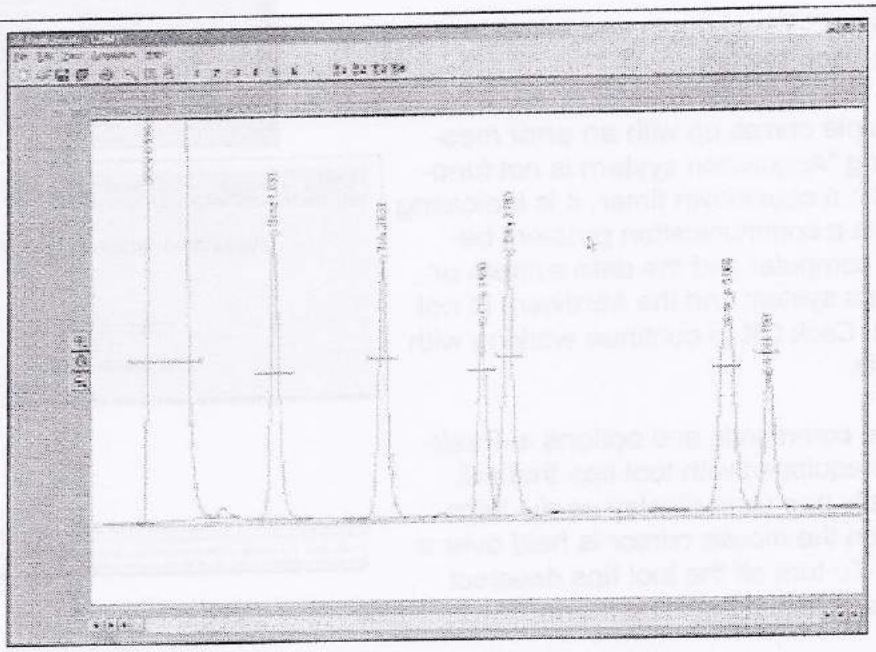


SRI Instruments

PeakSimple 2000

Chromatography Integration Software

Basic Tutorial



Installing PeakSimple 2000 from floppy disk or CD-Rom

A. Start the Windows operating system in use on your computer. (Windows 95, 98, ME, 2000)

B. Insert the PeakSimple 2000 disk or CD into your floppy disk drive.

C. Go to the **Start** menu in the bottom left hand corner of the windows screen and select **Run** from the set of icons.

D. From the run menu, type **X:\setup** (where **X** is the letter of your computers disk drive).

E. Now click on the **Continue** button with your mouse cursor or press the enter key on your keyboard to begin installation.

F. To complete installation follow the onscreen instructions provided by the installation wizard.

Installing PeakSimple 2000 from software download

A. Start the Windows operating system and use an online browser to access www.srigc.com.

B. From the menu on the left hand side of the screen select **Download our Software** and then download PeakSimple 2000 from the following page.

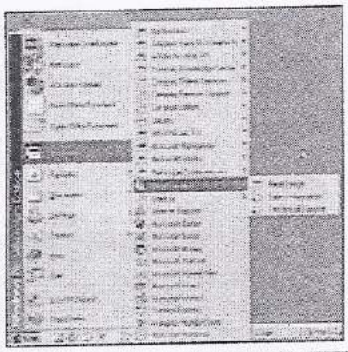
C. Save the file to a temporary folder and then double click on it from My Computer to allow the program to self-extract.

D. Once all the files have been extracted successfully double-click the install file and press the **Continue** button when prompted.

E. Follow the onscreen instructions to complete the installation of PeakSimple.

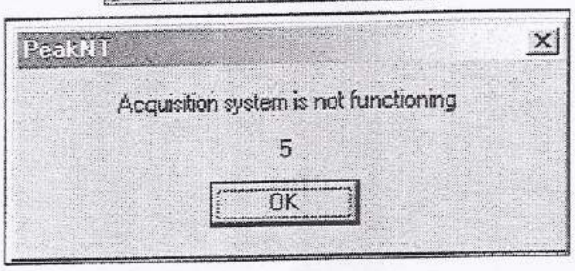
SRI Instruments 20720 Earl Street Torrance, CA 90503 U.S.A
Telephone: (310) 214-5092 Fax: (310) 214-5097 sales@srigc.com **www.srigc.com**

Launching PeakSimple 2000

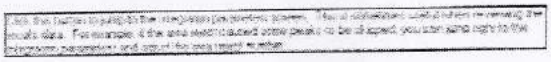


1. Click on the windows **Start** button in the bottom left-hand corner of the screen. Select **Programs** and then **PeakSimple** from the list of program groups on the screen and then click on **PeakSimple.**

2. This will launch PeakSimple and initialize the data acquisition system.

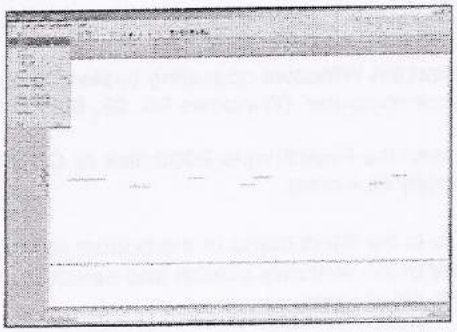


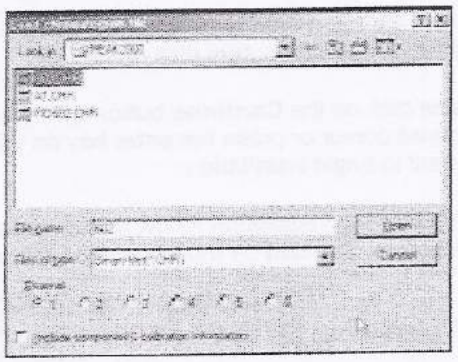
3. If PeakSimple comes up with an error message stating "Acquisition system is not functioning" with a countdown timer, it is indicating that there is a communication problem between the computer and the data system or that the data system and the hardware is not connected. Click **OK** to continue working 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.

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.

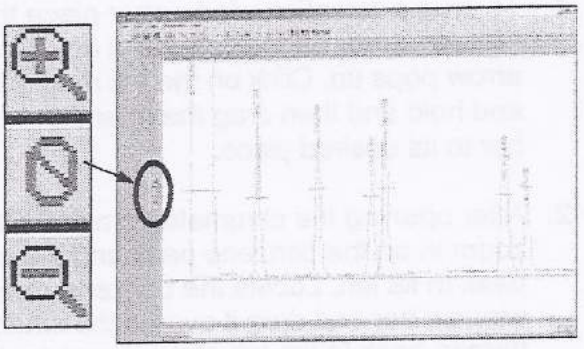
2. The Load Chromatogram File window is now open. The PeakSimple software includes a number of sample chromatogram data files that can be opened, displayed, and manipulated. One file, 602.CHR, will be used throughout the rest of the tutorial. Select file **602.CHR** from the PeakSimple directory, choose **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.

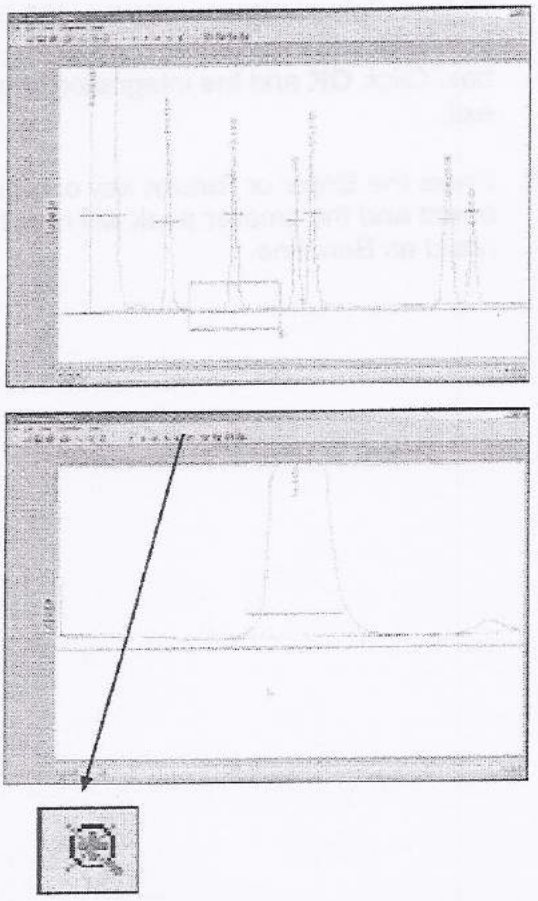


Zooming

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

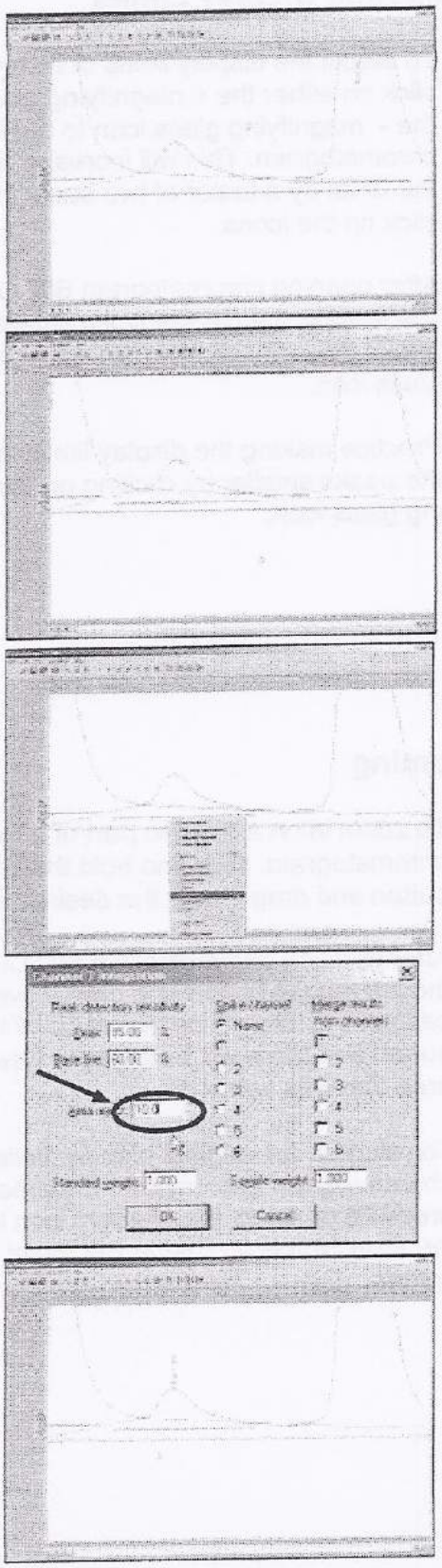
1. To drag a retention window bar place the mouse cursor on the bar until a double sided arrow pops up. Click on the left mouse button and hold and then drag the retention window bar to its desired place.

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.

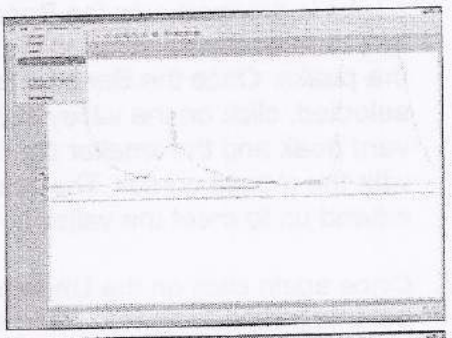
4. From the integration window locate the **Area Reject** dialogue box, erase the 100.0 in the box, and add the number **10.0** to the dialogue box. Click **OK** and the integration window will exit.

5. Press the **Enter** or **Return** key on your keyboard and the smaller peak will now be recognized as Benzene.

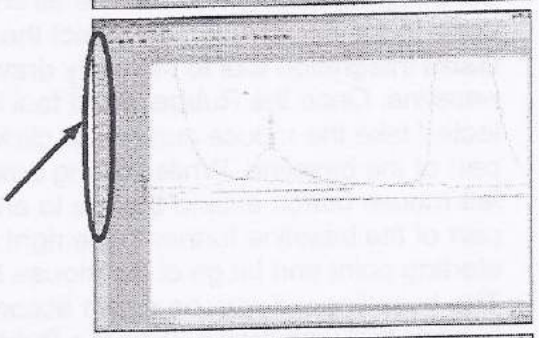


Manual Integration

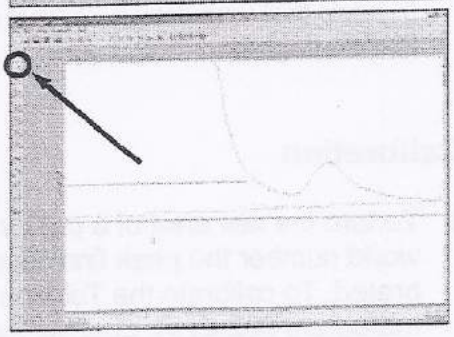
1. To manually adjust the integration baseline and peak separation in a chromatogram use the manual integration toolbar provided by PeakSimple. To open up the manual integration toolbar select **Edit** in the PeakSimple menu bar and then click on the **Manual Integration** option. The manual integration 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.

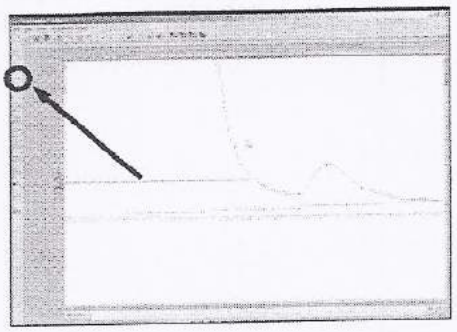


3. To make a baseline ignore a peak use the None integration tool. After opening chromatogram 602.CHR and the manual integration toolbar, zoom in on the baseline of the solvent peak and the smaller unrecognized peak immediately to its right. Click on the **None** integration tool in the manual integration 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.

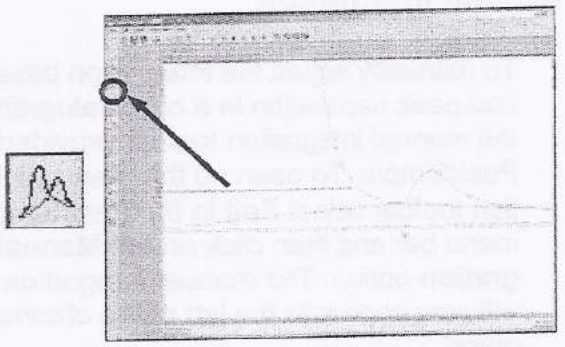


4. To undo the changes made to a chromatogram at any time simply click on the **Undo** integration tool in the manual integration toolbar. After selecting this tool all integration changes made to the chromatogram will be undone.

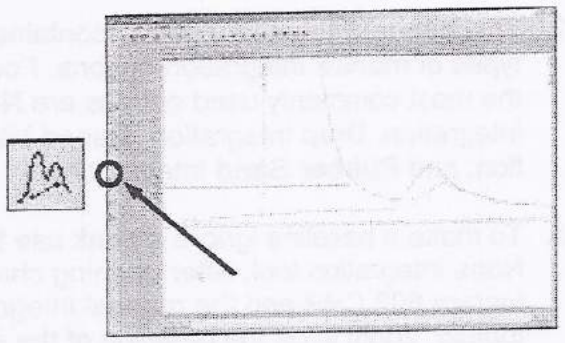
5. Click on the **Undo** tool with your mouse cursor and select the **Drop** integration tool to enable the dropping of the baseline below the between the two peaks. After selecting the Drop tool click where the valley of the peaks meet the baseline with the cursor. The baseline should now be dropped below the base of the peaks and a line should extend from it to the baseline.



6. 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.

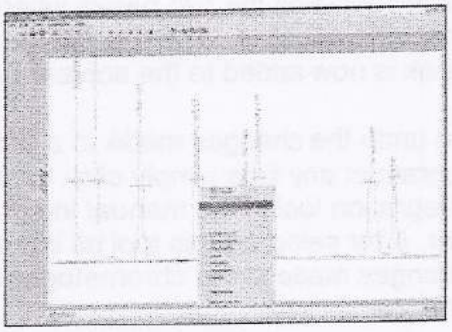


7. Once again click on the **Undo** tool in the manual integration toolbar to remove all changes done to the chromatogram. Select the **Rubber Band** integration tool to manually draw a baseline. Once the Rubber Band tool is selected take the mouse cursor and click on a part of the baseline. While holding 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.

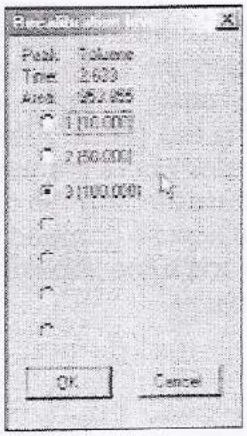


Calibration

1. 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.



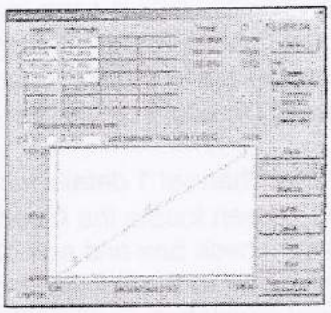
2. From the Recalibration level window click on the third level radio button **3 (100.000)** and then select **OK** with your mouse cursor.

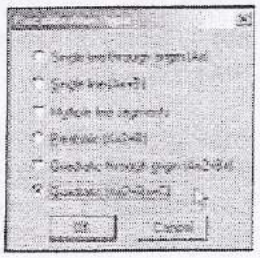


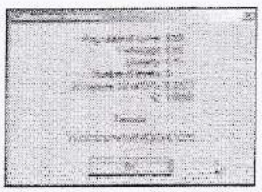
3. After selecting OK from the Recalibration level menu the Calibration menu for Toluene will pop up. Check to make sure the flashing asterisk on the calibration curve is on level 3 and then click on the **Accept New** button to the right of the window.

4. 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 (Ax2+Bx+C)** radio button and then click on **OK** with the mouse cursor.

5. 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.



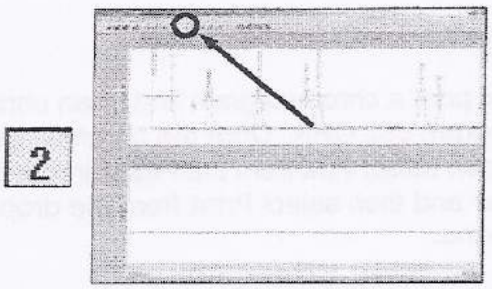


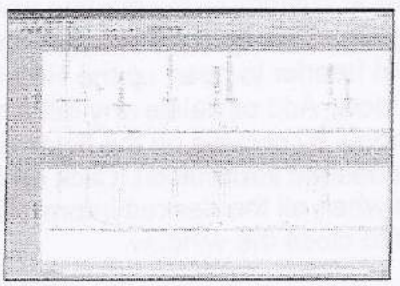


Overlay

1. 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.

2. 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.

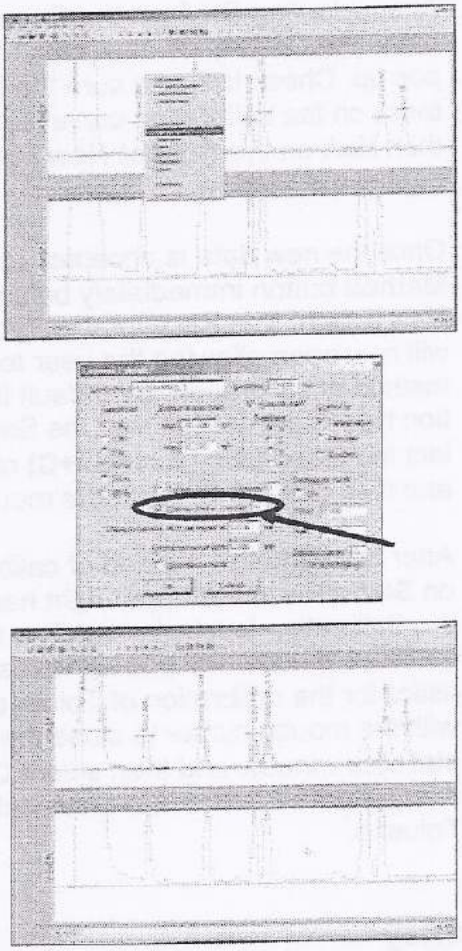




3. Once FID602.CHR is open in the second channel right click using the mouse on the chromatogram in the first channel and select **Channel Details** from the list of options.

4. 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.

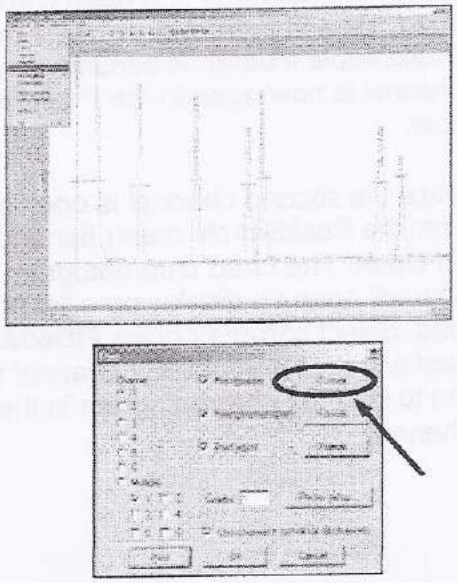
5. The chromatogram FID602.CHR is now in place overlaid on top of chromatogram 602.CHR in channel 1. Chromatogram 602.CHR is in blue while FID602.CHR is in red.



Printing a Chromatogram

1. 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.

2. 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.

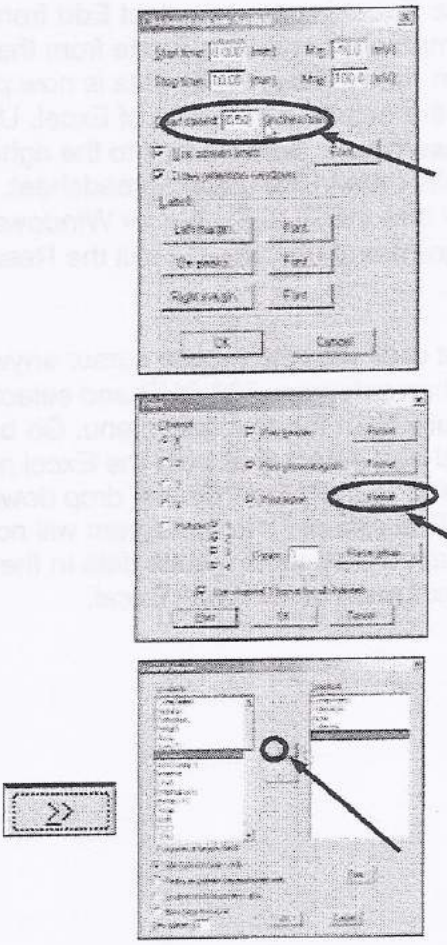


3. In the Print window click on the **Format** button for Print chromatogram to open up the Chromatogram format window. Locate the **Chart speed** dialogue box and insert the number of inches each minute on the chromatogram will take up when printed (for a nine minute run try **0.50** inches per minute).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

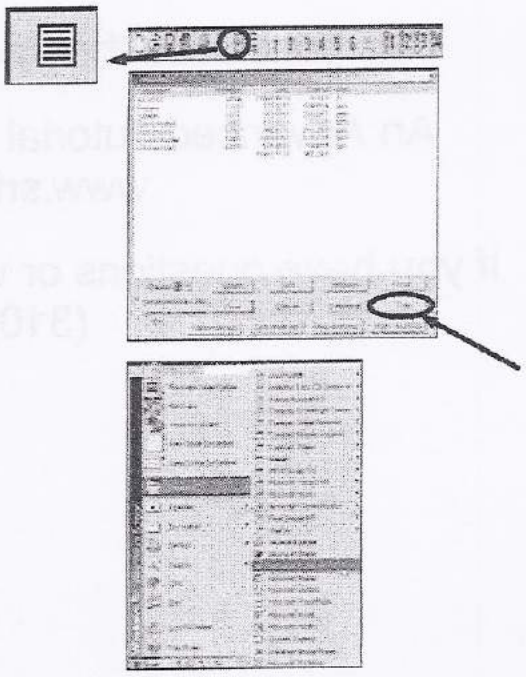
6. Select **Print** in the Print window to print the chromatogram or click on **OK** in the Print window to exit the window.



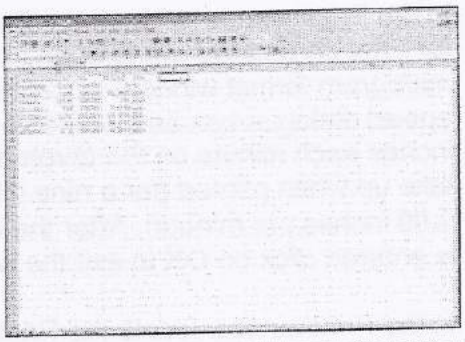
Exporting to Excel

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.

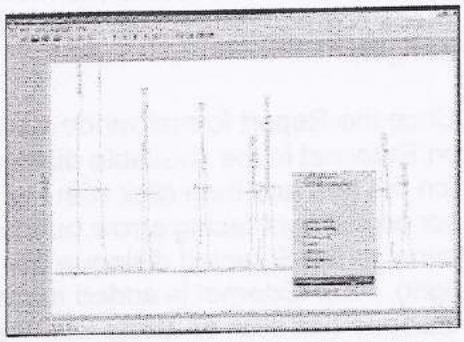
2. Make sure Microsoft Excel is loaded on the computer. If Excel is not loaded you can copy results data and chromatograms to Microsoft Word or PowerPoint. Open up Microsoft Excel by clicking with the mouse cursor on the **Start** button in the bottom left of the Windows screen and then **Programs**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

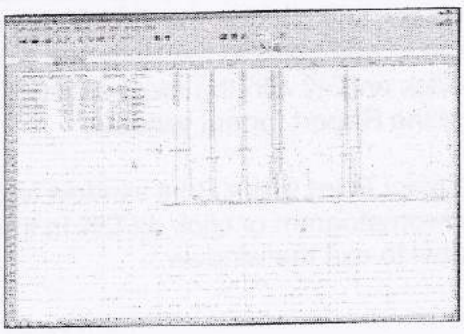


6. Once Excel is opened select **Edit** from the Excel menu bar and then **Paste** from the drop down menu. The results data is now placed into the columns and rows of Excel. Using the mouse cursor, select a box to the right of the results data in the Excel spreadsheet. Go back into the PeakSimple for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

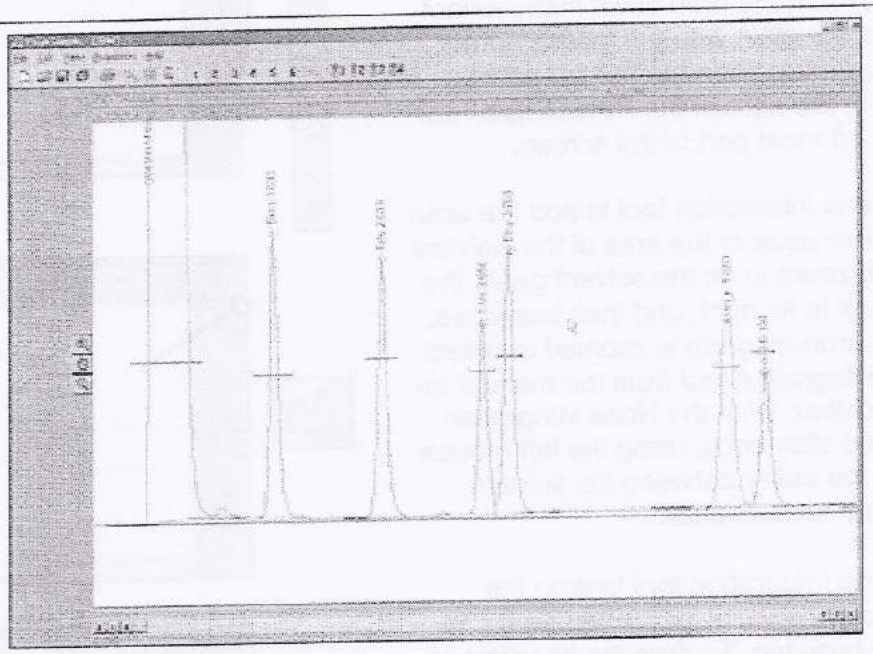
An Advanced Tutorial can be obtained by going to:
www.srigc.com online

If you have questions or would like to place an order call:
(310) 214-5092

PeakSimple 2000

Chromatography Integration Software

Advanced Tutorial



Installing PeakSimple 2000 from floppy disk or CD-Rom

A. Start the Windows operating system in use on your computer. (Windows 95, 98, ME, 2000)

B. Insert the PeakSimple 2000 disk or CD into your disk drive.

C. Go to the **Start** menu in the bottom left hand corner of the windows screen and select **Run** from the set of icons.

D. From the run menu, type **X:\setup** (where **X** is the letter of your computers disk drive).

E. Now click on the **Continue** button with your mouse cursor or press the enter key on your keyboard to begin installation.

F. To complete installation follow the onscreen instructions during the installation wizard.

Installing PeakSimple 2000 from software download

A. Start the Windows operating system and use an online browser to access www.srigc.com.

B. From the menu on the left hand side of the screen select **Download our Software** and then download PeakSimple 2000 from the following page.

C. Save the file to a temporary folder and then double click on it from My Computer to allow the program to self-extract.

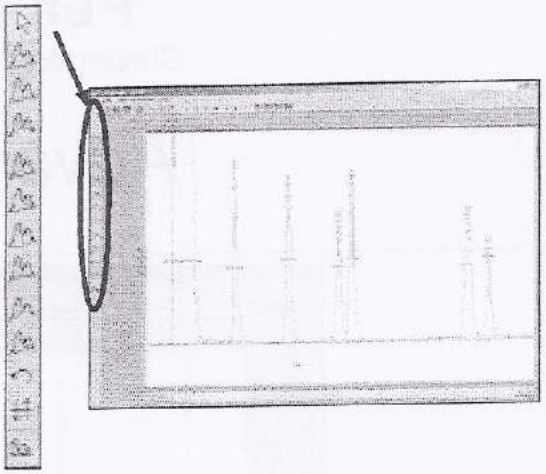
D. Once all the files have been extracted successfully double-click the install file and press the **Continue** button when prompted.

E. Follow the onscreen instructions to complete the installation of PeakSimple.

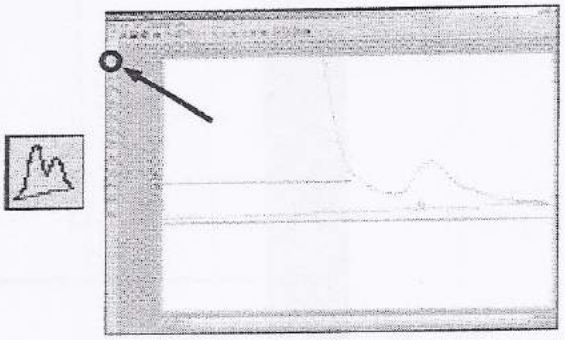
SRI Instruments 20720 Earl Street Torrance, CA 90503 U.S.A
Telephone: (310) 214-5092 Fax: (310) 214-5097 sales@srigc.com **www.srigc.com**

Manual Integration

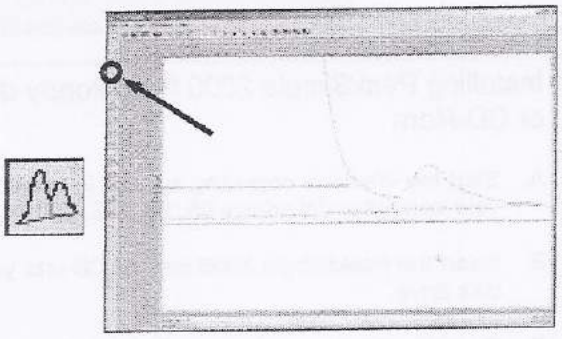
1. To manually integrate the PeakSimple baseline in a chromatogram use the manual integration tools found in the manual integration toolbar. To open the manual integration toolbar first have chromatogram 602.CHR loaded and then select **Edit** from the PeakSimple menu bar. From the drop down menu select **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.



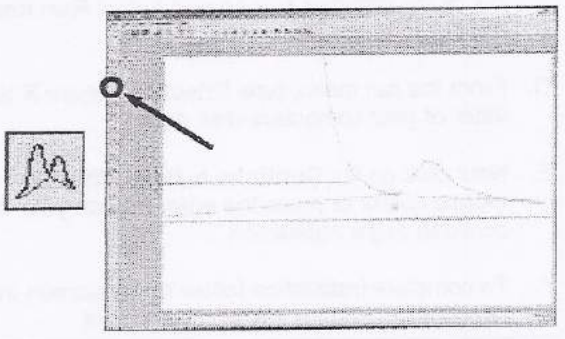
2. Use the None integration tool to add the area of the smaller peak to the area of the Solvent peak. First, zoom in on the solvent peak, the smaller peak to its right, and their baselines. Once the chromatogram is zoomed in select the **None** integration tool from the manual integration toolbar. With the None integration tool selected click once, using the left mouse button, on the valley between the solvent peak and the smaller peak.



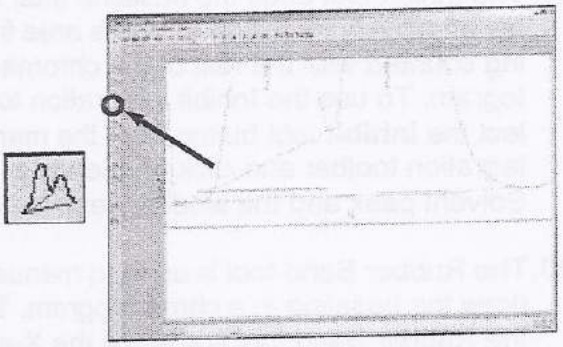
3. Use the Drop integration tool to drop the baseline from the valley of the two peaks to an existing baseline. To drop the baseline select the **Drop** integration tool from the manual integration toolbar. Using the mouse cursor, click on the valley between the solvent peak and the smaller peak to drop the baseline.



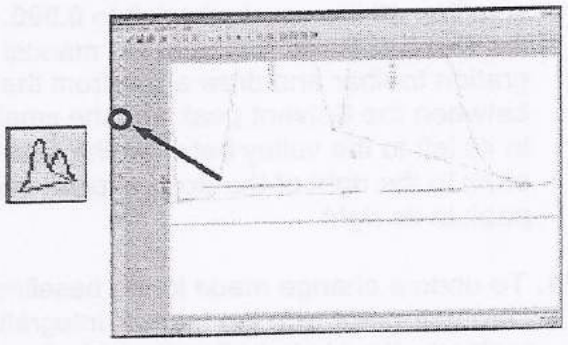
4. The Based integration tool raises the baseline to the valley between two specified peaks. With the baseline dropped, click on the **Based** integration tool button and then click on the valley between the solvent peak and the smaller peak to its right to raise the baseline to the valley.



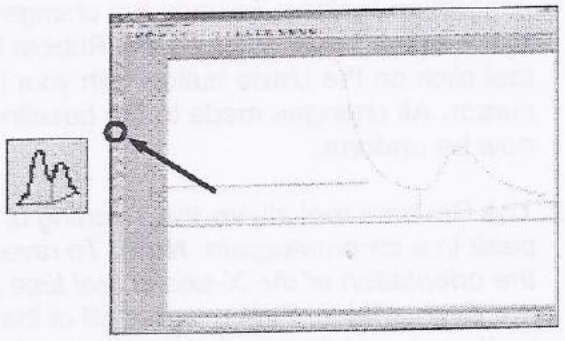
5. The Lead skim integration tool allows a peak's area to be skimmed off of the leading edge of another peak. To use the Lead skim tool first unzoom off of the solvent peak and the other smaller peak and then zoom in on the Chlorobenzene peak, the Ethylbenzene peak, and the baseline. After the chromatogram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



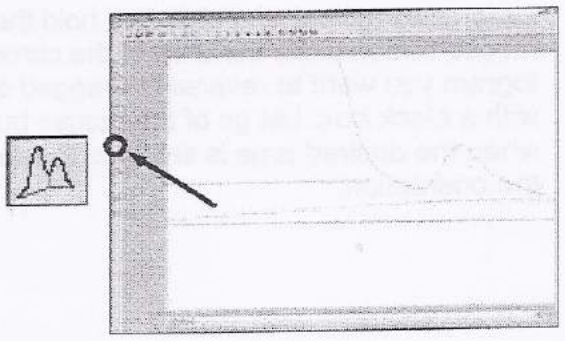
6. The Trail skim integration tool is similar to the Lead skim tool except a peak's area is now skimmed off of the trailing edge of another peak. Select the **Trail skim** tool button from the manual integration toolbar and then click on the valley between the Chlorobenzene and Ethylbenzene peaks with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



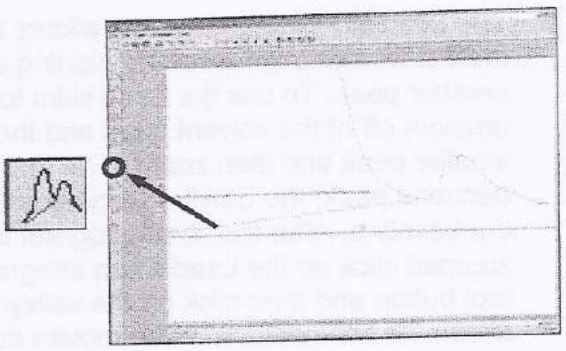
7. The Lead horizontal tool constructs the baseline horizontally for the leading peak while the trailing peak's baseline stretches from the horizontal line to the next valley. Unzoom off of the Chlorobenzene and Ethylbenzene peaks and instead zoom in on the Solvent peak, the smaller peak to its right, 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.



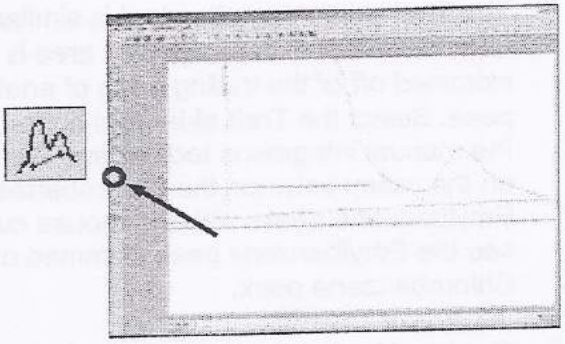
8. The Trail horizontal integration tool drops the baseline horizontally for the trailing peak while the lead peak's baseline stretches from the horizontal line to the previous valley in the chromatogram. After selecting the **Trail horizontal** tool in the manual integration toolbar click with the mouse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

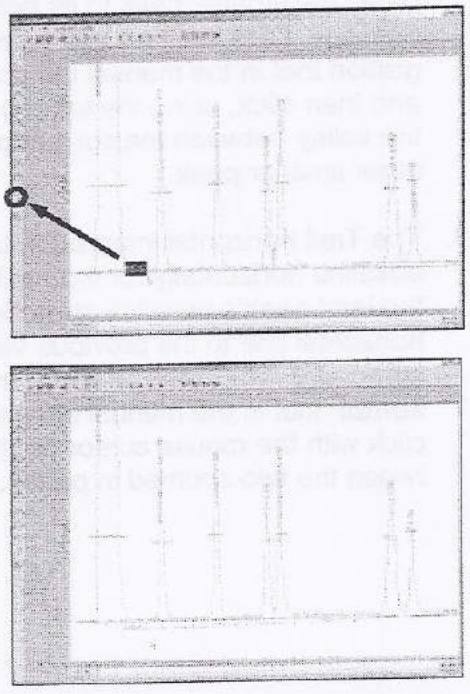


10. The Rubber Band tool is used to manually draw the baseline in a chromatogram. To use the Rubber Band tool first scroll the X-axis scrollbar all the way to the left to **0.000**. Select the **Rubber Band** tool from the manual integration toolbar and draw a line from the valley between the Solvent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

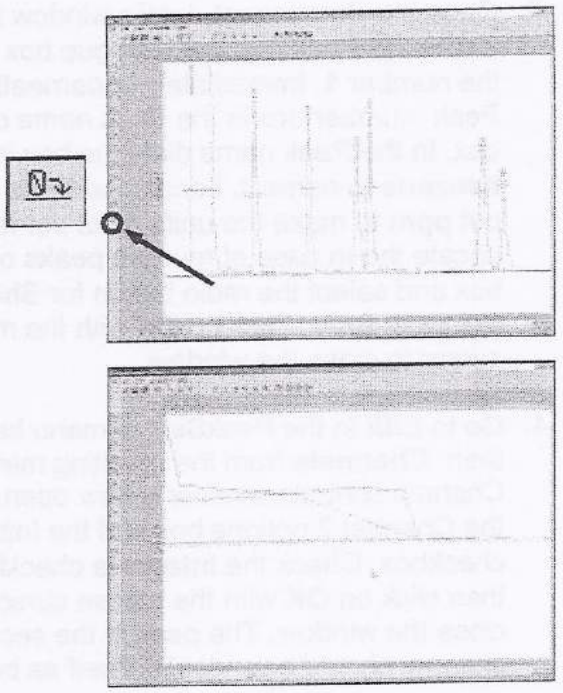


11. To undo a change made to the baseline of a chromatogram with the manual integration tools use the Undo button found in the manual integration toolbar. To undo the changes made to the baseline using the Rubber band tool click on the **Undo** button with your mouse cursor. All changes made to the baseline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



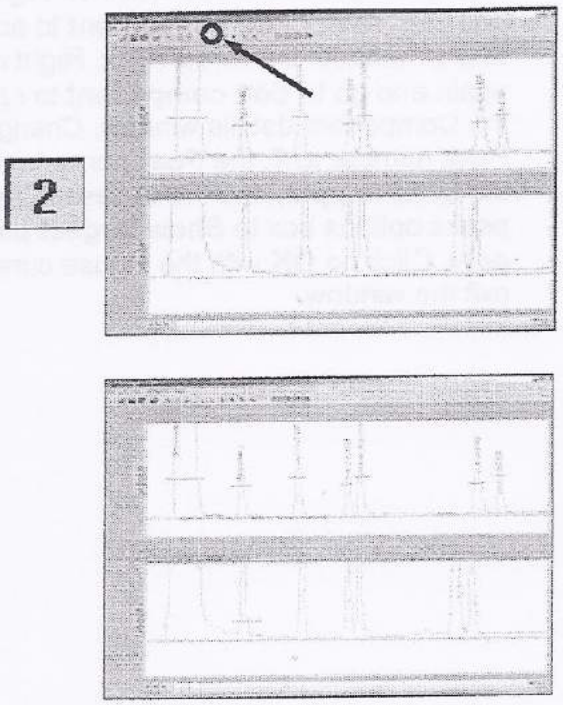
13. The Zero tool is used to set the value of the data line at a selected point and following in the chromatogram to zero. First undo the changes done to the chromatogram by the Reverse tool by reopening 602.CHR in the PeakSimple menu bar. ***Note:*** *Changes made to a chromatogram by the Reverse tool 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.



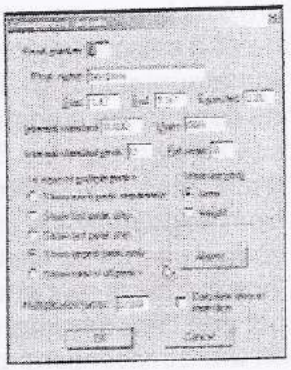
Creating Component Tables

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.

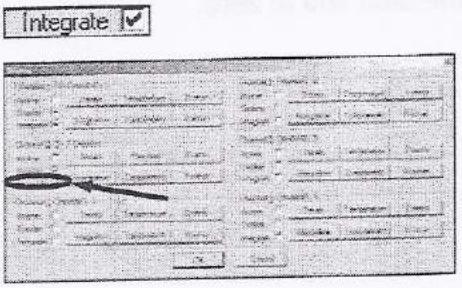
2. In channel 2 locate the second tall peak from the left and right click on it with the mouse cursor. From the resulting menu select **Add component** to add a retention window bar to the peak. Once again right click on the peak and select **Edit component** from the menu to open up the Component details window.



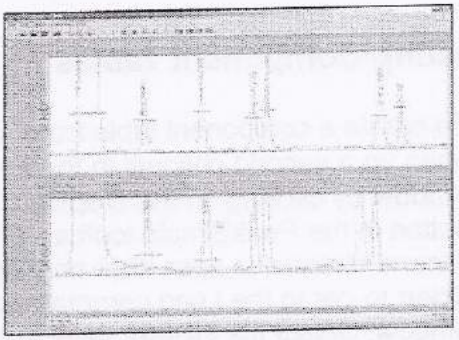
3. Once the Component details window is open locate the Peak number dialogue box and add the number **1**. Immediately underneath the Peak number box is the Peak name dialogue box. In the Peak name dialogue box input **benzene** to name it. Locate the Units box and put **ppm** to make the units parts 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.

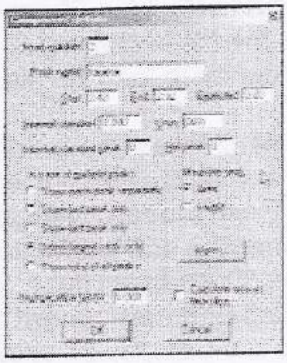


4. Go to **Edit** in the PeakSimple menu bar and then **Channels** from the resulting menu. The Channel controls window is now open. Locate the Channel 2 options box and the Integrate checkbox. Check the **Integrate** checkbox and then click on **OK** with the mouse cursor to close the window. The peak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

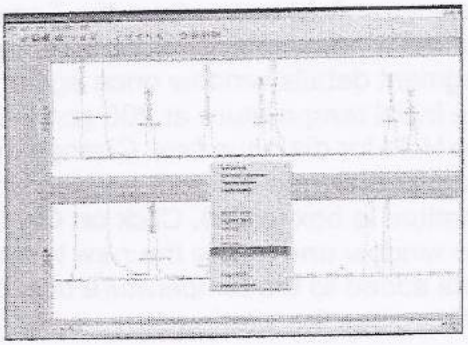


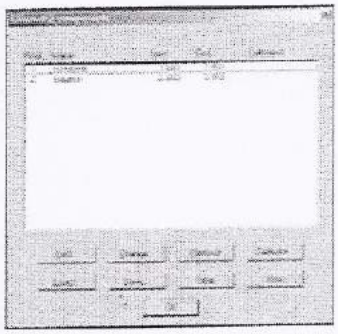
5. Locate the large peak to the right of the benzene peak in the second channel. Right click and then select **Add component** to add a retention window bar to the peak. Right click again and go to **Edit component** to open up the Component details window. Change the Peak number to **2**, the Peak name 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.





7. 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.

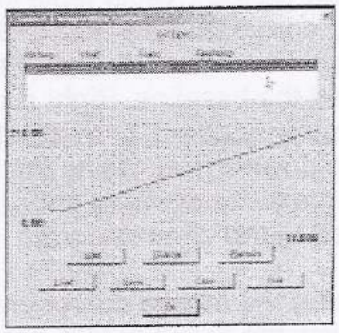


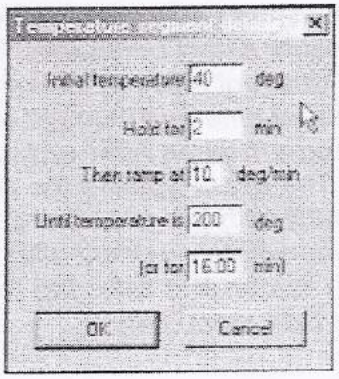


Temperature Programming

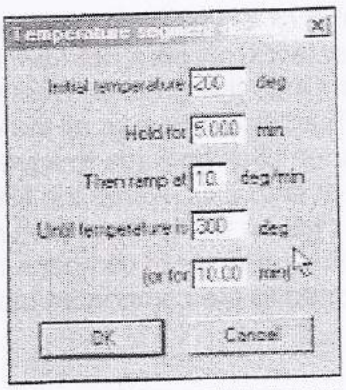
1. To modify the temperature programming in PeakSimple first open chromatogram 602.CHR and then right click anywhere on the chromatogram. From the drop down menu select **Temperature** to open up the Temperature control window.

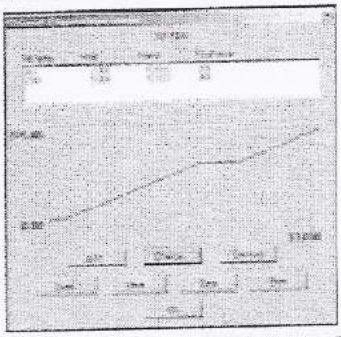
2. In the Temperature control window click using the mouse cursor on the set of numbers in the box and select **Change** from the group of buttons below. The Temperature segment details window will open allowing the modification of the temperature programming. Locate the Hold for dialogue box and insert a **2** in the box. Click on **OK** to close the window and go back into the Temperature control window.





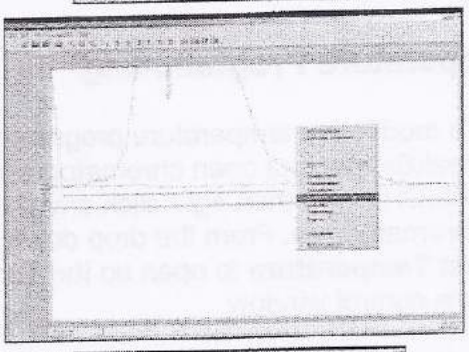
3. Select the **Add** button from the Temperature control window to open up the Temperature segment details window once again. Leave the Initial temperature at 200 and insert a **1** in the Hold for dialogue box. Change the Then ramp at dialogue box to **5** and the Until temperature is box to **250**. Click on **OK** to close the window and to see the new temperature data added to the temperature box. Click on **OK** to close the window.



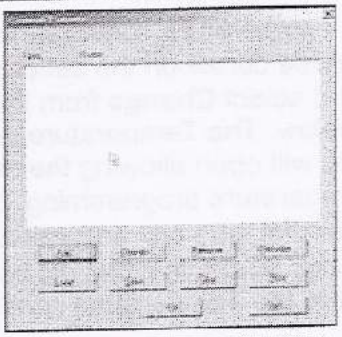


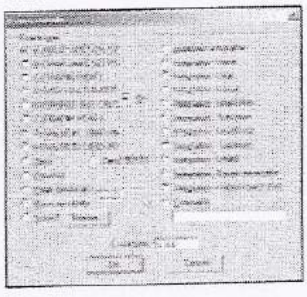
Events Table

1. To modify up the Events table in PeakSimple open up chromatogram 602.CHR and zoom in on the benzene peak, the smaller peak to its right, and the baseline. Right click anywhere on the chromatogram and select **Events** from the drop down menu. Doing this will open up the Events window where specific events can be added to the chromatogram.

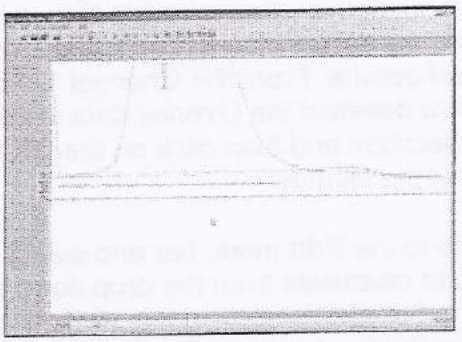


2. Click using the mouse cursor on the **Add** button to view the Event details window. A list of event types are available with their radio buttons to either select or deselect the event. ***Note:*** *The event types to the left of the window are real-time and thus will only affect the chromatogram when AID hardware is connected. The event types to the right are concerned only with integration and their changes will be immediately evident after returning to the main screen and selecting* ***Reintegrate*** *from the* ***Edit*** *menu bar.*



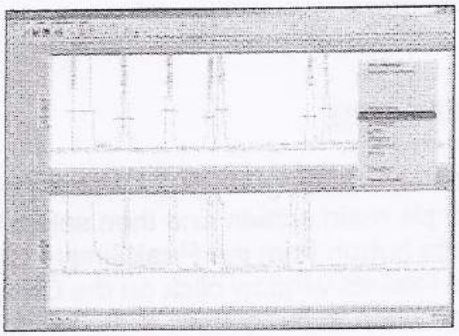


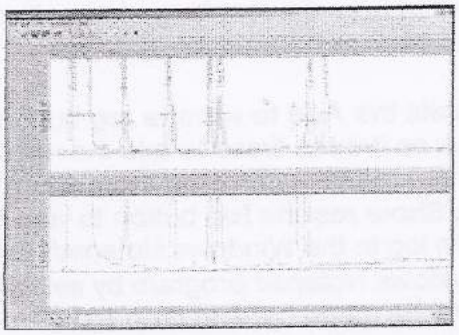
3. In the Event details window locate and select the relay **G** radio button with the mouse cursor and then locate the Event time dialogue box and enter **.1** in the box. Click on **OK** to exit the window. ***Note:*** *The relay might be used to actuate a valve when hardware is connected.* The event 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.



4. 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

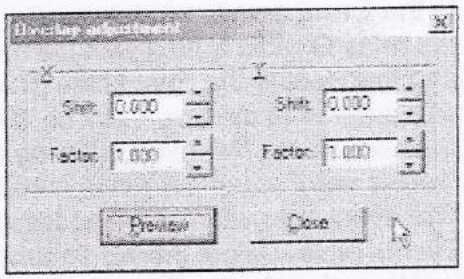




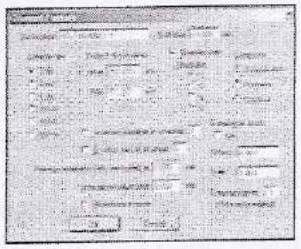
1. To overlay one PeakSimple chromatogram on top of another chromatogram open up a second channel in the main screen and load chromatogram 602.CHR in the first channel and chromatogram FID602.CHR in the second channel. Right click anywhere in the first channel and select **Channel details** from the drop down menu.

2. 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.

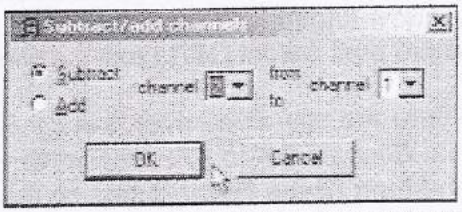
3. Right click anywhere on the first channel and select **Overlay adjustment** from the drop down menu. In the Overlay adjustment window locate the Factor scroll box in the X box. Experiment scrolling the X factor up or down to shift the overlaid chromatogram to its right or left. Locate the Factor scroll 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.

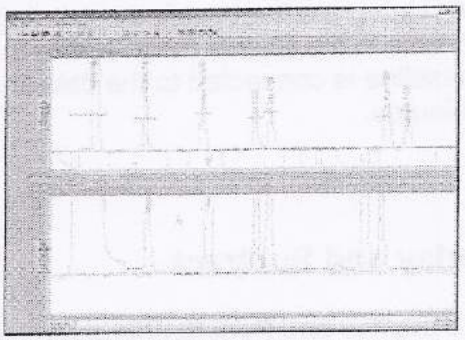


4. To subtract a chromatogram in one channel from another channel, right click using the mouse cursor on channel 1 and select **Channel details**. From the Channel 1 details window deselect the Overlay data in channel checkbox and then click on the **OK** button to exit the window.



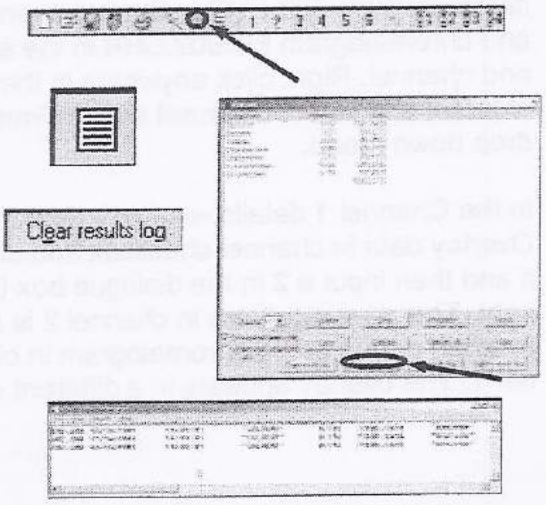
5. Go to the **Edit** menu bar and select **Subtract/ Add channels** from the drop down menu. In the Subtract/add channels window make sure the Subtract radio button is selected and that channel 2 is being taken from channel 1. Click on the **OK** button to make the changes take effect and have channel 2 subtracted from channel 1. The normal way to use this feature is to subtract a drifting baseline from a chromatogram.





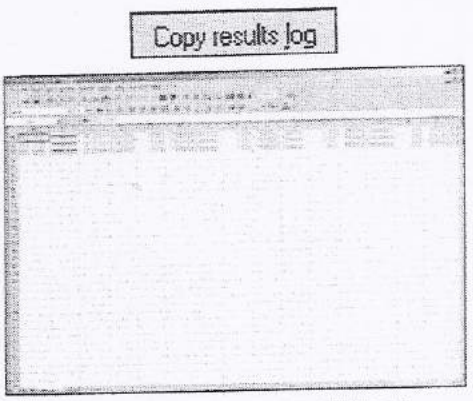
Results Log

1. 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.

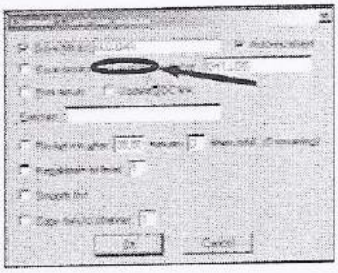


2. Locate the **Add to results log** button and click on it three times to add the results on the screen to the Results log three times. Click on the **Show results log** button to view the results log in the Windows Notepad. Exit the Windows Notepad program by selecting **File** from the menu bar and then **Exit**.

3. 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.



4. 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.

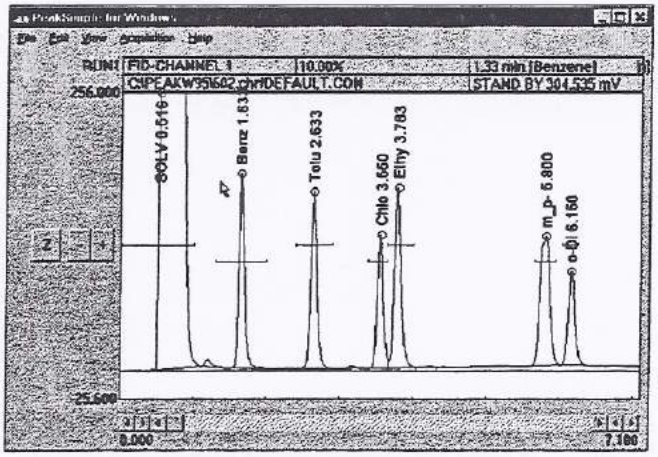


This concludes the PeakSimple 2000 Advanced Tutorial

Further documentation can be obtained by going to:
www.srigc.com online

If you have questions or would like to place an order call:
(310) 214-5092

PeakSimple for Windows Software and Chromatography Data System Validation Statement



February 1, 1999

1) PeakSimple for Windows software and Chromatography Data System (PeakSimple) is written, manufactured and maintained by SRI Instruments, Inc. a Nevada Corporation.

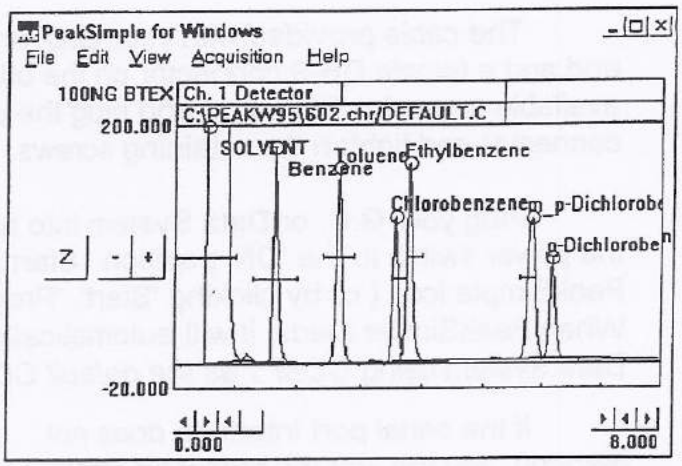
2) PeakSimple for Windows software has been under continuous development since 1994. Periodic testing of the software is performed by SRI employees.

3) PeakSimple software is designed to be self-validating to enable quick verification by customers that PeakSimple is functioning consistently, reliably and according to specifications under actual operating conditions.

4) Self-validation is performed by configuring PeakSimple into the "Loopback mode" (see loopback instructions in manual). In this mode, an actual user generated chromatogram which is loaded into channel 4 is re-played (like a tape recorder) through the TP2 output channel, and then re-acquired and processed through any one of the remaining input channels. This is done 7 or more times to insure that data is being processed consistently and reliably.
The results from multiple loopback analyses are used to calculate the percent relative standard deviation (precision) of each peak in the chromatogram. Chromatographic data is highly variable, and the precision obtained is dependent on many factors including the peak shape, signal to noise ratio, interferences, co-eluting peaks, data acquistion rate and customer selected integration parameters. For this reason, self-validation is more valid than factory validation, since self-validation takes into account the exact chromatographic conditions and user specified parameters in effect for the particular application whereas factory validation can not.

Getting Started

In this section, we will cover the basic information needed to set up proper communication with your G.C. or Data System hardware.
The Windows version of PeakSimple requires the use of the serial port interface that is built into most 8610-C and Model 310 gas chromatographs. This data acquisition and interface unit permits you to acquire up to four separate channels of data simultaneously without the need for additional hardware or acquisition boards.



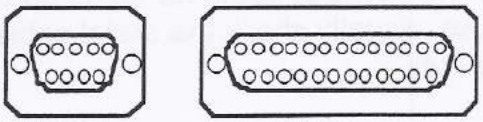
The earlier IBM PC-compatible ISA expansion bus data acquisition cards (AD100 and AD110) used by PeakSimple II and PeakSimple III data systems are *not supported* by PeakSimple for Windows. However, all chromatograms acquired using DOS-based PeakSimple II and PeakSimple III continue to be compatible with this Windows version and may be imported as native files.

Identifying Your COM Port

Before attempting to establish communication between your G.C. and the serial data system interface, be sure to check that all the necessary electrical connections have been made, including the connection of any optional remote start cables.

Select an unused serial port on your PC and identify the COM port number assigned to it. It is important that this port NOT SHARE AN INTERRUPT with any other device used in your computer. Typical PCs are equipped with two COM (or serial) ports. COM 1 is typically used by the mouse or some other pointing device. COM 2 may be open (unused) or shared with another device, such as a fax modem, scanner or other peripheral. Determine which COM port you will use and remove any other device that may be in contention with that specific COM port number. Refer to your PC's hardware manual for instructions on changing COM port addresses and device drivers.

Most COM ports are provided with DB-9 connectors (nine pins configured in two rows - 5 pins over 4 pins - within a D-shaped plug or chassis connector). If your PC has a DB-25 serial port (25-pin connector), you will require a DB-25 to DB-9 adapter.



DB-9 Serial Port Connector

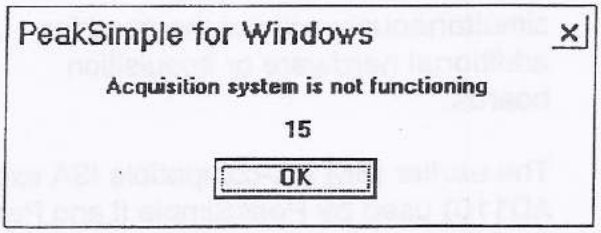
DB-25 Serial Port Connector

Establishing Communication

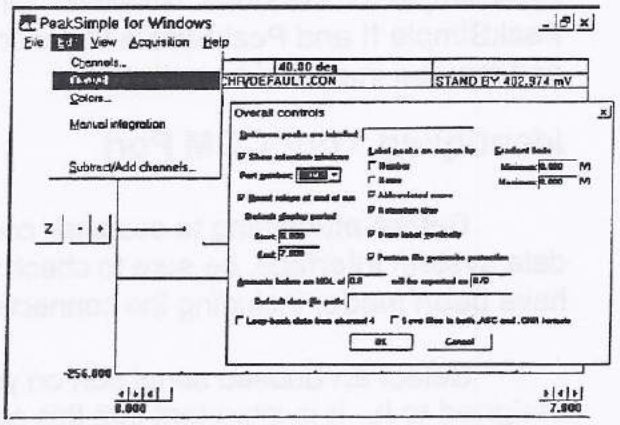
The cable provided with your G.C. or data system has a male DB-9 plug on one end and a female DB-9 connector on the other end. Plug one end of this cable into your available computer COM port and plug the other end into the G.C. or Data System DB-9 connector and tighten the retaining screws.

Plug your G.C. or Data System into an approved GFCI protected outlet and turn the power switch to the 'ON' position. Start PeakSimple by double-clicking on the PeakSimple icon (or by clicking 'Start', 'Programs', 'PeakSimple' in Windows 95). When PeakSimple loads, it will automatically attempt communication with your G.C. or Data System using *COM 1 as the default COM port.*

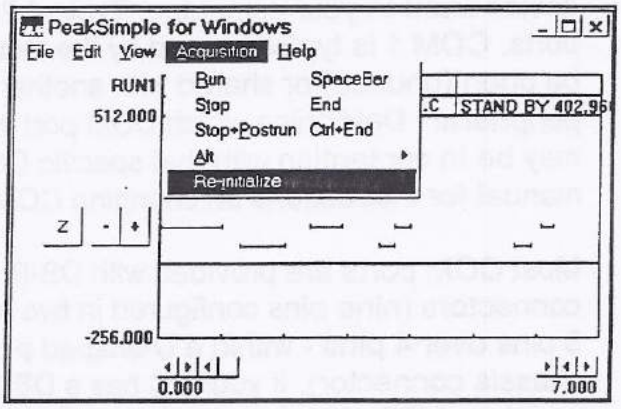
If the serial port interface does not respond, you will see the following error messages appear on the screen: **"Can't wake- check power and cable"** followed by the message **"Acquisition system is not functioning".**



These messages indicate that your computer cannot communicate with your G.C. or Data System through the default COM port, COM 1. You will need to set up the correct COM port in PeakSimple. To do this, click on the **EDIT** pull-down menu and select **OVERALL**. Change the **PORT NUMBER** to the COM port into which you chose to plug your interface cable. Click **O.K.**.



If at anytime you wish to force PeakSimple to reinitialize communication, click on the **ACQUISITION** pull-down menu and select **RE-INITIALIZE**. If the COM port information is correct and communication errors still appear when the computer attempts to activate the serial port interface, check the serial port connections at both ends of the interface cable for loose connections. Also, visually check the serial cable for nicks or cuts.

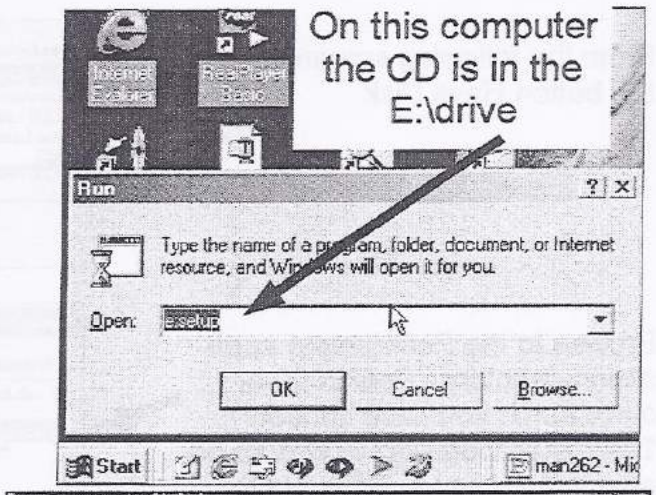


It is important to understand that in order for PeakSimple to communicate with your G.C. or Data System, at least ONE channel must be **ACTIVE**. To determine which channels are active, click on the **EDIT** pull-down menu and select **CHANNELS**. A channel is active if the box next to **ACTIVE** is marked with a checkmark. The **EDIT-CHANNELS** menu is described in greater detail in the **EDIT** section in this manual.

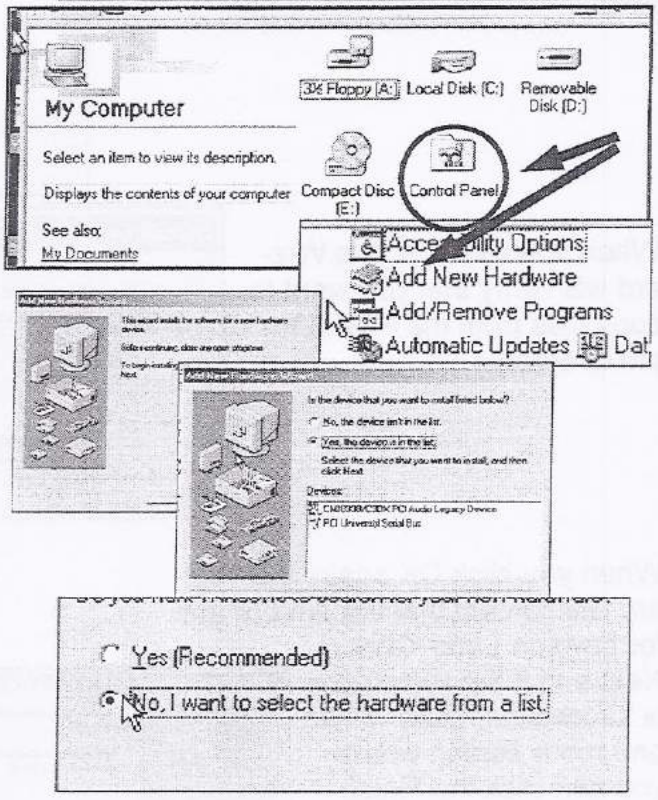
Chapter: PeakSimple

Topic: Installation of USB drivers for use with Model 302 USB data system

Install PeakSimple software from the installation CD or from a download from SRI's website http://www.srigc.com. The download is a zip file which must be un-zipped using PKZip or Win-Zip. From the Windows RUN command click on setup.exe in either the CD drive or the directory where the download was saved.



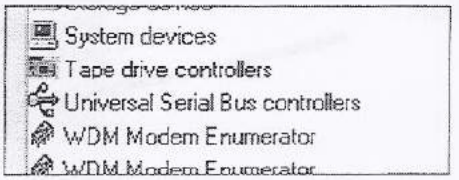
At the conclusion of the PeakSimple software installation, there will be 3 important files saved to the application directory. The application directory could be c:\Peak2000 or it could have another name which you specified during the installation. The 3 import files are named LL_USB.inf, LL-USB.sys and LL_USB2K.sys. These files are required to make Windows recognize the A/D board connected to the USB port of the computer.



Click on the Windows My Computer icon and then Control Panel and then on Add New Hardware.

Click on the NEXT button several times until you get to the screen which allows you to select hardware from a list.

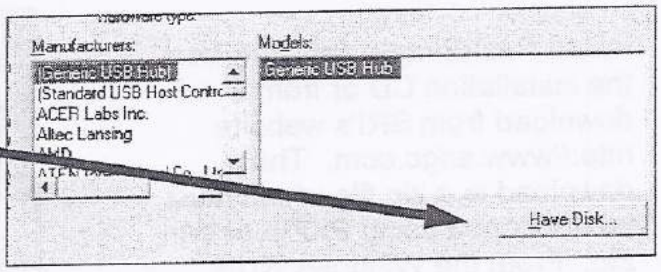
Scroll down the list until you can click on Universal Serial Bus controllers



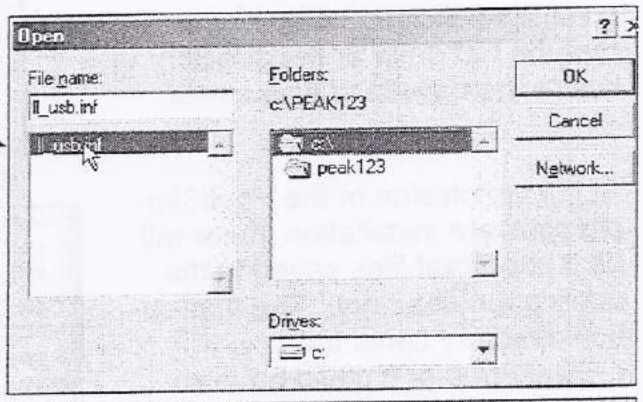
Chapter: PeakSimple

Topic: Installation of USB drivers for use with Model 302 USB data system

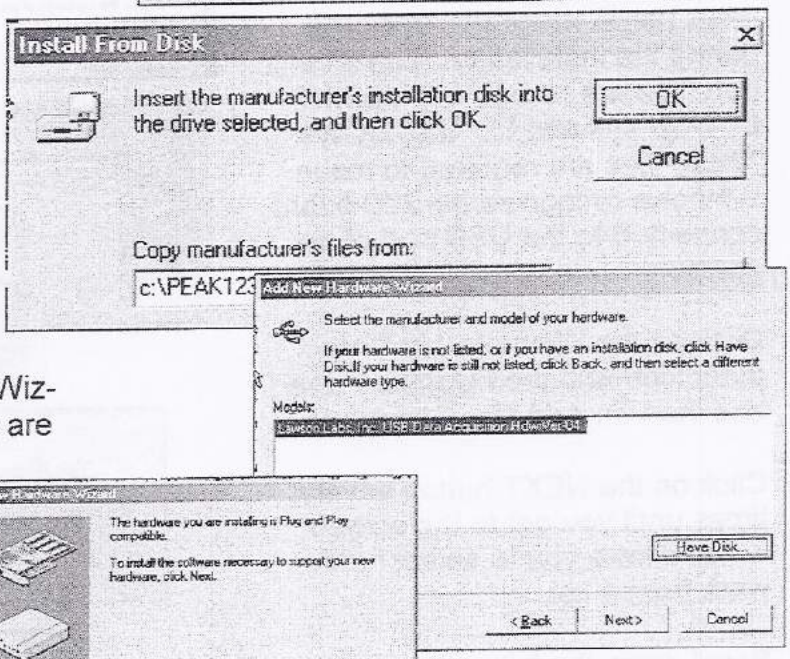
From the following screen click on the button Have Disk



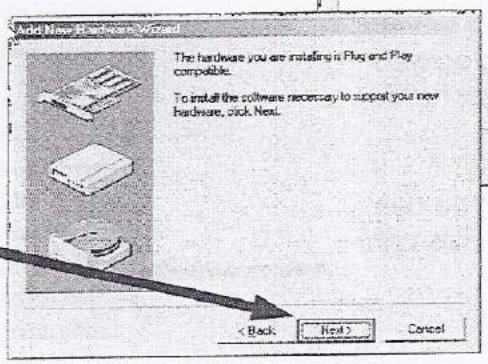
Browse to the PeakSimple application directory (Peak2000 or other name you have chosen). The Installation Wizard should be able to find the LL_USB.inf file.



When you click OK, the Wizard will verify that you want to copy files from the PeakSimple directory.



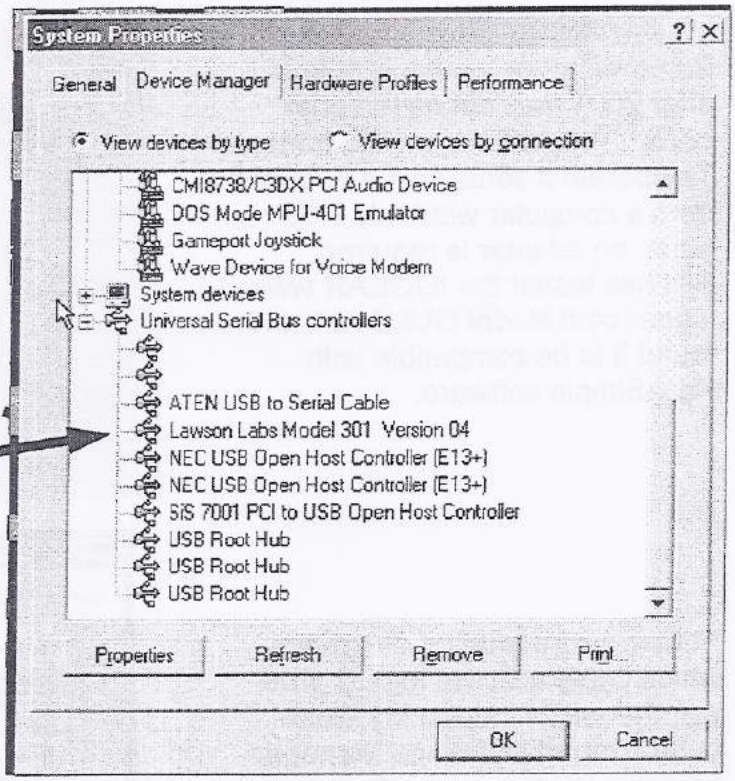
When you click OK again, the Wizard will confirm that the drivers are for Lawson Labs. Click Next and if the installation is successful, there will be one more screen where you can click the Finish button.



Chapter: PeakSimple

Topic: Installation of USB drivers for use with Model 302 USB data system

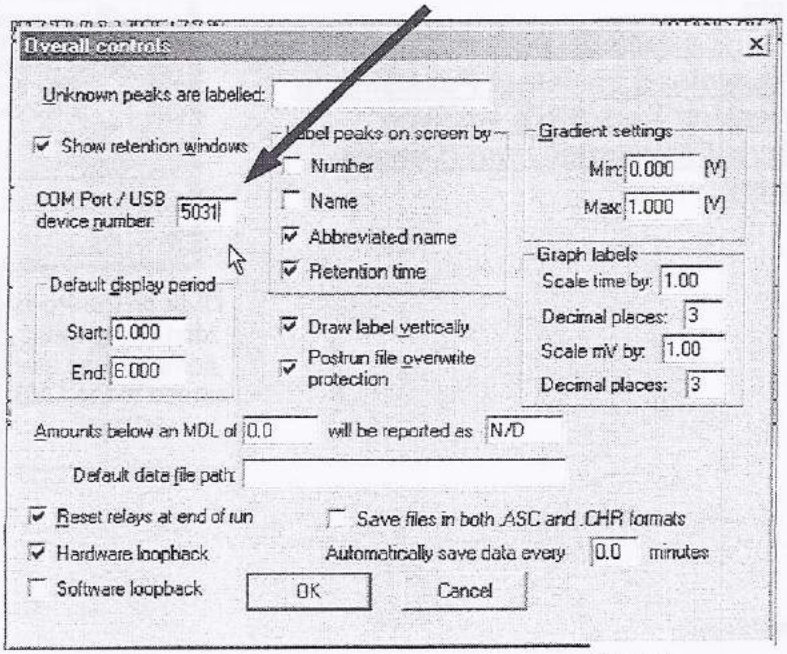
You must RESTART the COMPUTER before the drivers will work.



Once the computer has restarted right click on My Computer and examine the System/Device Manager Screen. If the USB drivers have been successfully installed, the Universal Serial Bus Controllers section will list Lawson Labs Model 301 version 04.

You can now launch PeakSimple. Each USB data system has a unique USB device number which must be entered into the Edit\Overall window in PeakSimple. The USB device I.D. is listed on the back of each GC or stand-alone data system and will be a 4 digit number starting with 5 (5031, 5032, etc.) Once you enter the number PeakSimple will attempt to wake up the data system. Don't forget to click the SaveAll icon so you don't have to re-enter the USB device I.D. again.

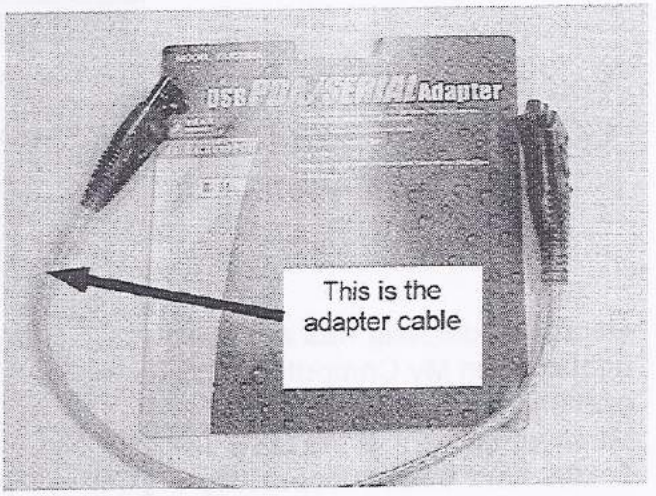
Enter the USB device I.D. number in PeakSimple's Edit/Overall screen.



Chapter: PeakSimple

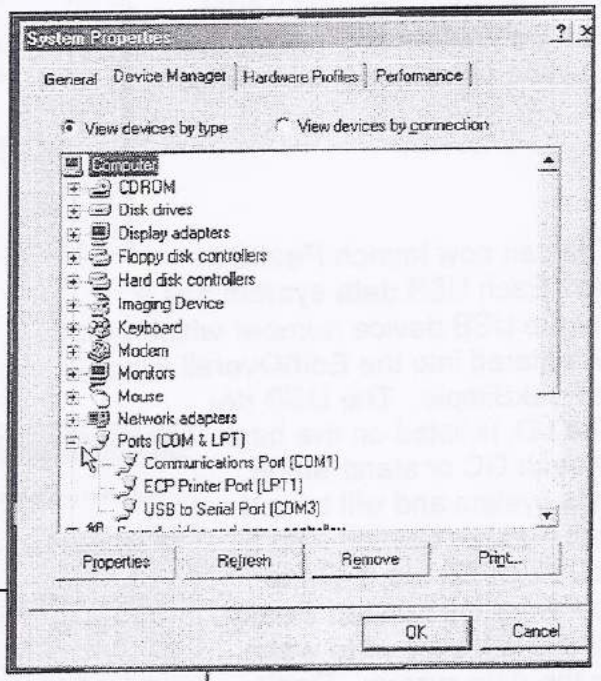
Topic: Operation of serial port Models 203 and 202 on computers with USB ports only

Some Windows computers sold after 2001 may not have serial ports. They will have USB ports. To operate a serial port A/D board from a computer with only USB ports, an adapter is required. SRI has tested the IOGEAR www.iogear.com Model GUC232A and found it to be compatible with PeakSimple software.



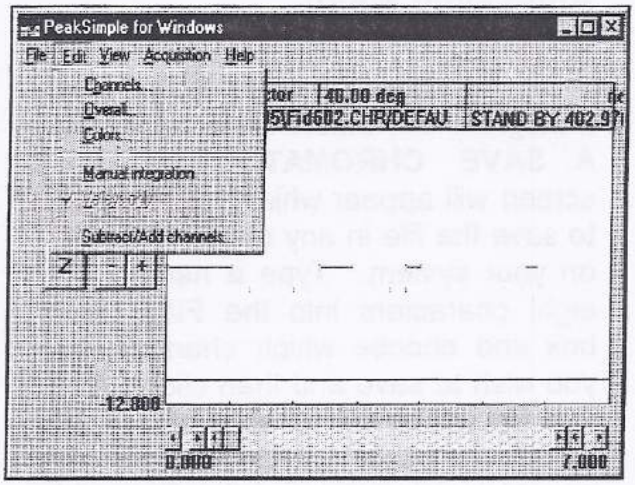
Follow the installation directions which come with the logear product, then examine the My Computer/Properties\Device Manager screen and click on the Ports icon. The serial port may be assigned to Com 5 which is only supported by version 2.83 and later PeakSimple.

Download the latest PeakSimple version from SRI's website http://www.srigc.com if necessary



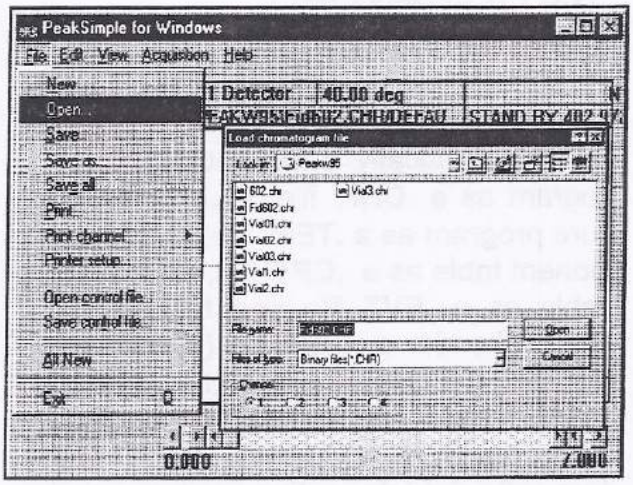
Click on the Ports icon to see what comport was assigned to the USB adapter

Operation of Menu Bar Pull-Down Menus



All PeakSimple for Windows features may be accessed from pull-down menus. When you click on a menu bar item, a pull-down group menu will open to permit navigation to specific group features. These pull-down menus may also be opened by pressing the **<ALT>** key and the letter key corresponding to the **underlined** letter in the menu bar item name. For example, to open the **EDIT** menu press **<ALT>** and the letter "E" (This is not case sensitive).

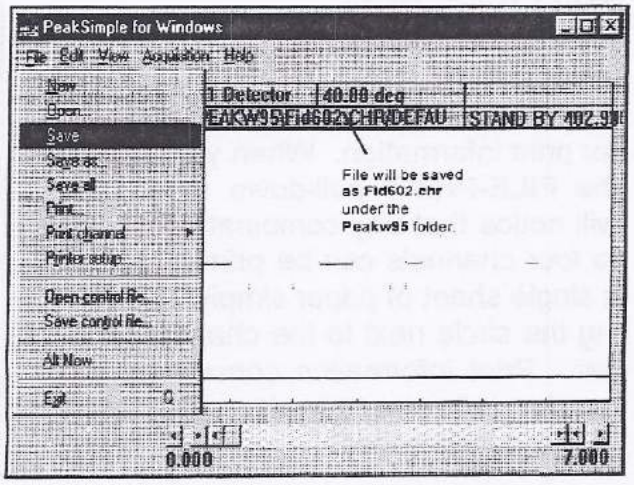
The FILE Pull-Down Menu



The **FILE-NEW** feature will clear the display of all active channels in the **Main** timebase without starting a new chromatographic run.

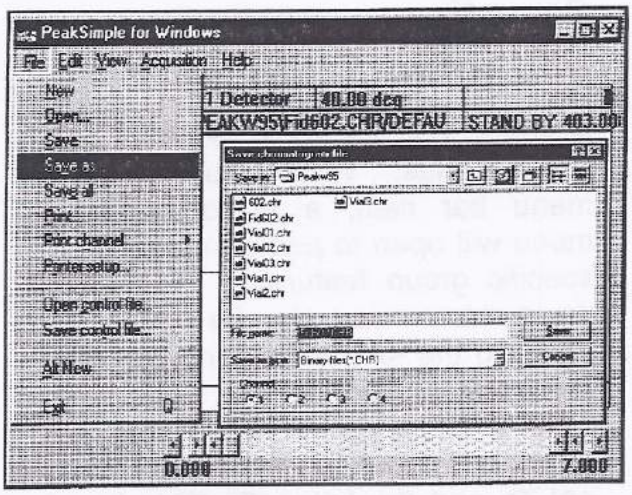
To open a previously saved chromatogram file, select **FILE-OPEN**. A **LOAD CHROMATOGRAM FILE** screen will appear which will allow you to select any file from any directory (folder) on your system. Choose the channel (1-4) in which you wish to display your saved chromatogram and than click **OPEN**.

FILE SAVE



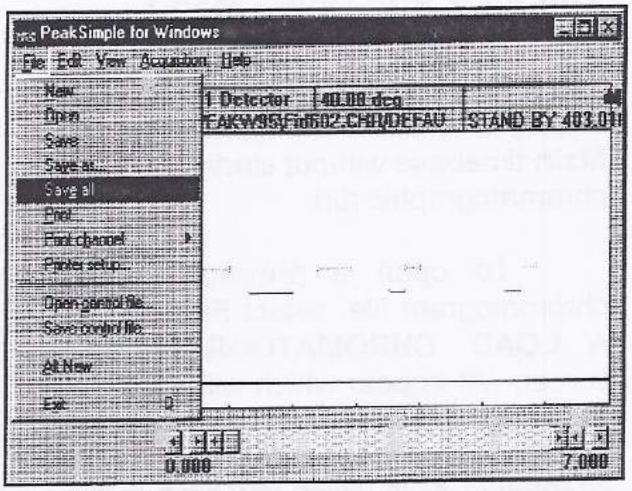
The **FILE-SAVE** feature saves the displayed chromatograms of all active channels. The name given to the file(s) is the same name that is displayed in the Data Boxes below the menu bar and will be given the default **.CHR** extension. This file name is editable by the user by changing information in the **EDIT-CHANNELS-POSTRUN** pull-down menu. See the **EDIT** section for more information.

The FILE-SAVE-AS Pull-Down Menu



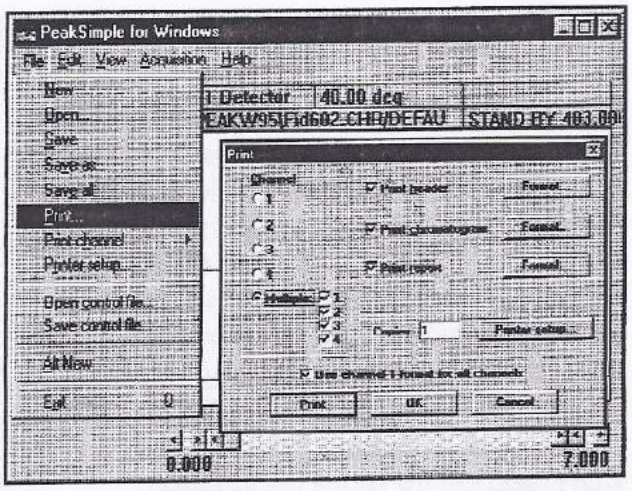
To save a newly created chromatogram file, select **FILE-SAVE AS**. A **SAVE CHROMATOGRAM FILE** screen will appear which will allow you to save the file in any directory (folder) on your system. Type a name up to eight characters into the **File** Name box and choose which channel (1-4) you wish to save and than click **SAVE**. The file will be saved as a **binary file** by default, with a **.CHR** extension. You may also select to save the file in **ASCII** format with a **.ASC** extension.

The FILE-SAVE-ALL Pull-Down Menu



The **FILE-SAVE-ALL** feature will automatically save your chromatogram as a **.CHR** file; your temperature program as a **.TEM** file; your component table as a **.CPT** file; your event table as a **.EVT** file and then saves them all under a control file (**.CON** file). **DEFAULT.CON** will be used if no other name for the **control file** is specified using the **SAVE-CONTROL FILE** feature. All print information is also saved when you save a **control file**.

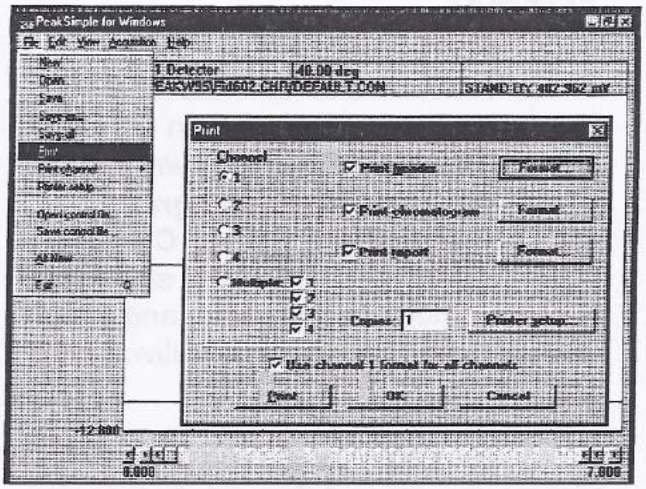
The FILE-PRINT Pull-Down Menu



Numerous fields are available for print information. When you access the **FILE-PRINT** pull-down menu you will notice that any combination of one to four channels can be printed out on a single sheet of paper simply by marking the circle next to the channel number. Print information concerning the **header, chromatogram** and **report** can be easily edited.

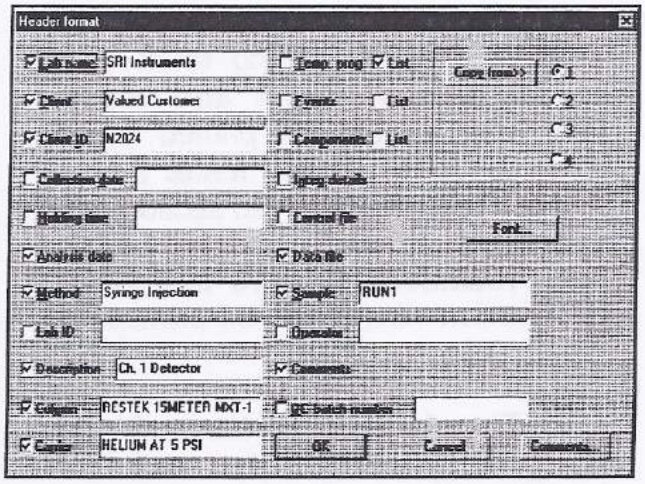
The FILE-PRINT Pull-Down Menu (CHANNEL 1)

When you access the **FILE-PRINT** pull-down menu you will notice that you can select to print any combination of **multiple** channels by clicking on the circle next to the word **multiple.** You may also choose to print individual channels by clicking on the circle next to the desired channel. **Click on Channel 1** to edit the **Channel 1** information in the **Print Header, Print Chromatogram and Print Report Format** fields. Rather than enter unique information for all four channels, you may wish to check the **Use channel 1 format for all channels** box.

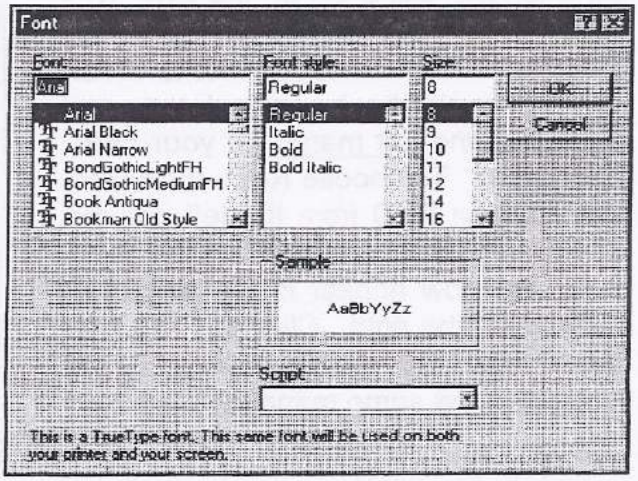


PRINT HEADER FORMAT

Clicking on the **Print Header FORMAT** button will allow you to customize the appearance of your printed chromatogram header. Input your **Laboratory name**, **Analysis method, Sample type, Column, etc** and check the box next to each field. **Analysis date** prints the date in your PC's BIOS.



Print out **Temperature Programs, Events and Components** file names by checking their boxes; or click on **List** to print the complete Temperature Program, Event Table or Component List. **Copy from:** selects which channel will provide the **List** information. Check the **Comments** box and click on **Comments...** to enter customized information about your analysis. You can change the **Font,** style and size of your printed text by clicking on the **Font** box. Select a size that will provide readable text while still leaving room for your chromatogram and report.

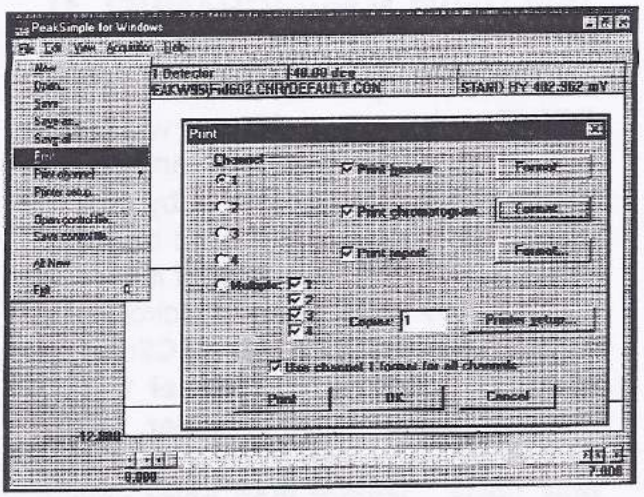


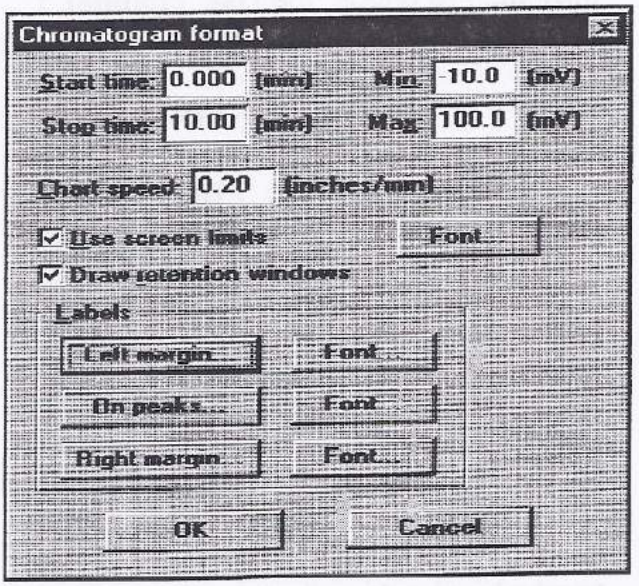
PRINT CHROMATOGRAM FORMAT

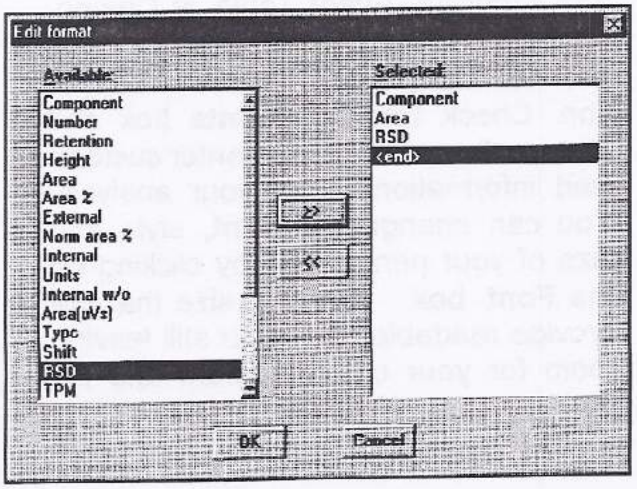
You can also edit the chromatogram print parameters when you access the **FILE-PRINT** pull-down menu. Check the **Print Chromatogram** box and select **Format**. The **Chromatogram format** screen allows editing of the chromatogram **Start time** and **Stop time** and the **Min** and **Max** millivolt levels.

The **Chart speed** setting will determine the size of the chromatogram section of your printout. A setting of **1.0 inches/minute** for a 5 minute chromatogram will produce a **5 inch** chromatogram print. You may need to experiment with this setting to fit your **header, chromatogram and report** information all on one printed page. When the **Use screen limits** box is checked only the displayed section of a chromatogram will be printed. The **Draw retention windows** box allows for retention windows to be printed as well.

The **Labels** section of the screen lets you select what useful information will be printed along the borders of the chromatogram, and above the peaks. Clicking on **Left margin**, for example, will bring up the **Edit format** screen which will allow you to select from a list of measurements which will automatically be calculated and printed in the left margin of your chromatogram. To choose **RSD**, for example, click on **RSD** from the left column and then click on the right arrows (>>). **RSD** will now appear in the **selected** column on the right. Click **OK** to close the window. Edit **On peaks** and **Right margin** in the same manner.

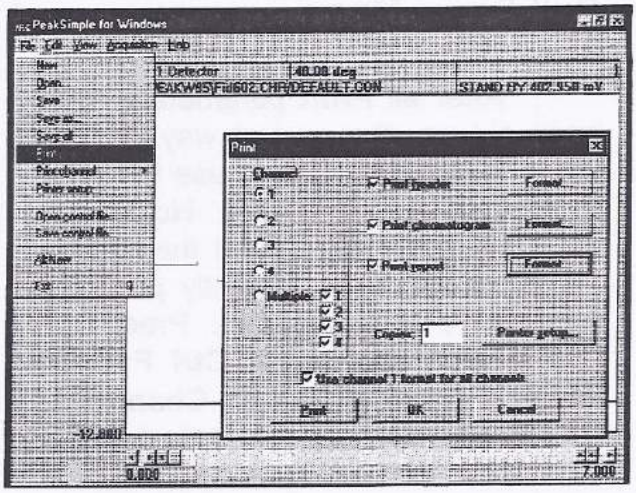




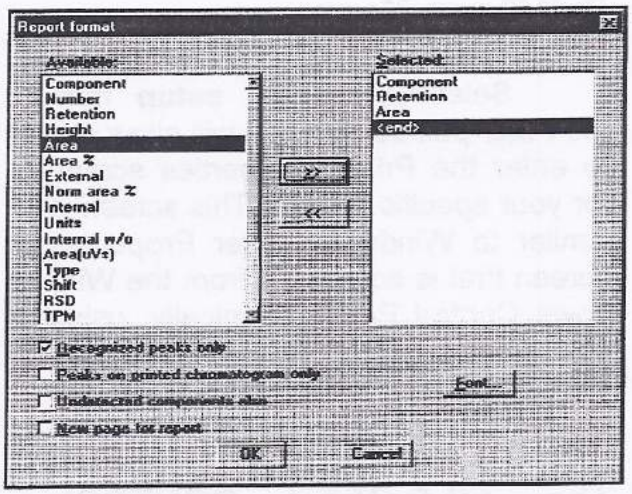


PRINT REPORT FORMAT

A report may be printed along with your chromatogram to summarize component retention time, area counts or other data. Clicking on the **View** pull-down menu and selecting **Results** will show a preview of your report.

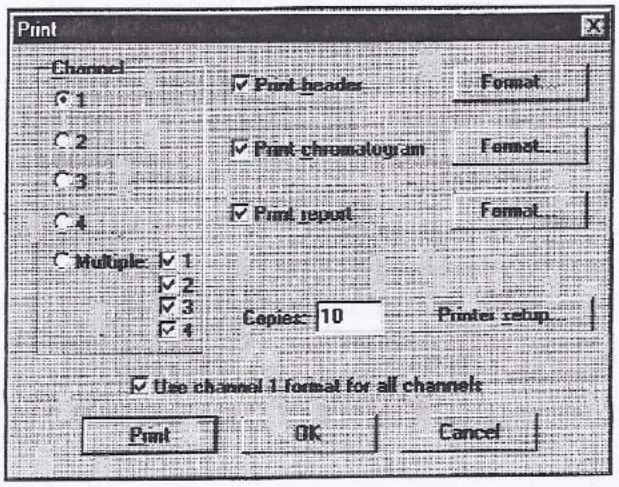


Click on the **Print Report** box and select **Format**. The **Report Format** screen will appear which will allow you to select from a list of measurements which will automatically be calculated and printed on the bottom of your chromatogram. To choose **AREA**, for example, click on **AREA** from the left column and then click on the right arrows (**>>**). **AREA** will now appear in the **Selected** column on the right.

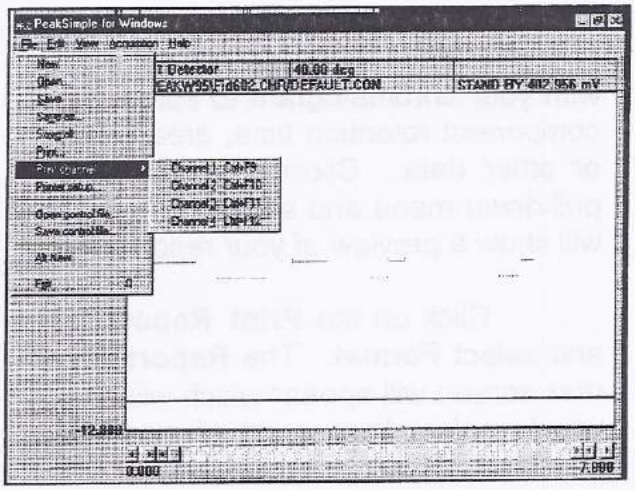


Clicking on the box next to **Recognized peaks only** will place a check mark in the box and only those peaks which integrate properly within named retention windows will be printed in the report. Checking the **Peaks on printed chromatogram only** box will allow the report to show only those peaks defined by the **Chromatogram format– Start time and Stop time.** This feature allows you to set up your report to ignore all peaks that appear outside your window of interest.

Checking the **Undetected components also** box will report information about all named peaks even if no peak is present within the retention window. Checking **New page for report** will print all report information on a separate page. Click **OK** to close the **Report format** window. You may print out as many Chromatogram **Copies** as you need by entering a number in the **Copies** box and selecting **Print**.

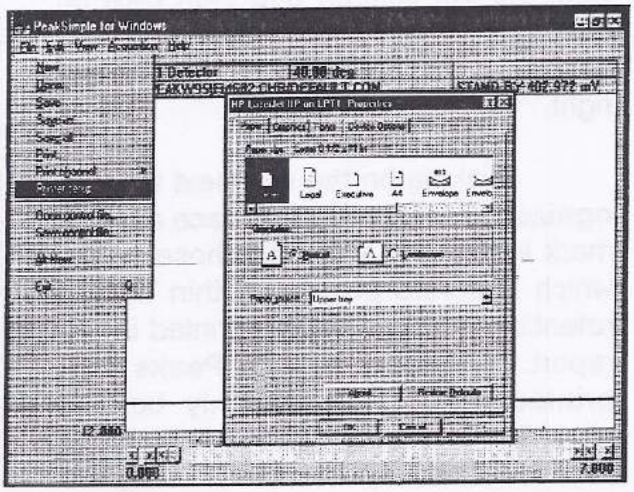


The FILE-PRINT CHANNEL Pull-Down Menu



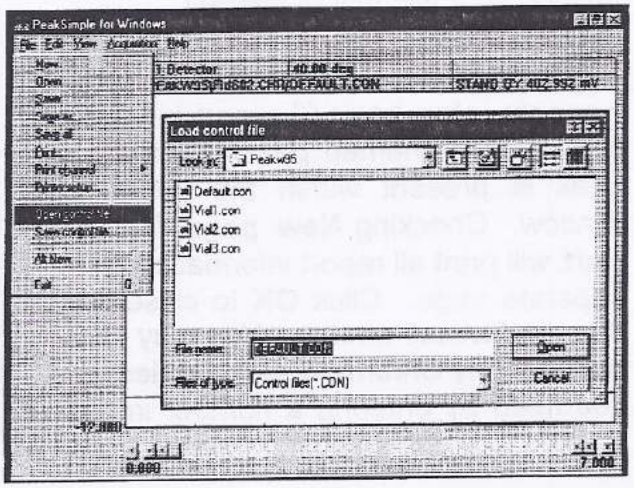
After all **Print** parameters have been set up, the easiest way to print out a chromatogram is to use the **File-Print Channel** quick keys. Hold down the **Ctrl** (control) key and then press **F9** (function #9) to instantly print the **Channel 1** chromatogram. Press **Ctrl F10** to print **Channel 2, Ctrl F11** for **Channel 3** or **Ctrl F12** for **Channel 4**. Of course you may also select these commands from the pull-down menu.

The FILE-PRINTER SETUP Pull-Down Menu



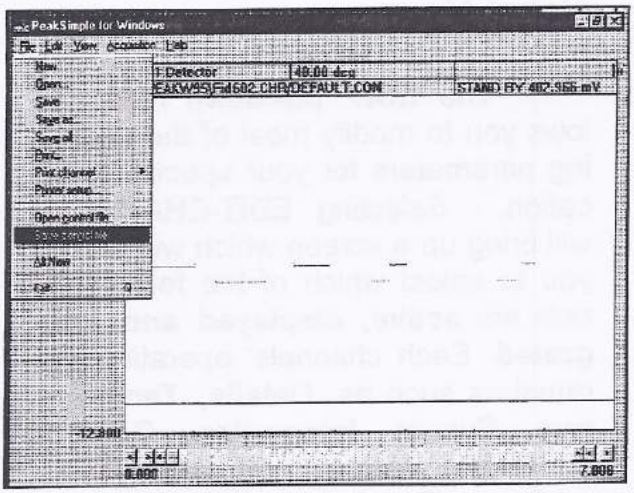
Selecting **Printer setup** from the **FILE** pull-down menu will allow you to enter the Printer Properties screen for your specific printer. This screen is similar to Windows Printer Properties screen that is accessible from the Windows Control Panel. Typically, using your printer default settings with **portrait** orientation will produce a visually appealing printout.

The FILE-OPEN CONTROL FILE Pull-Down Menu

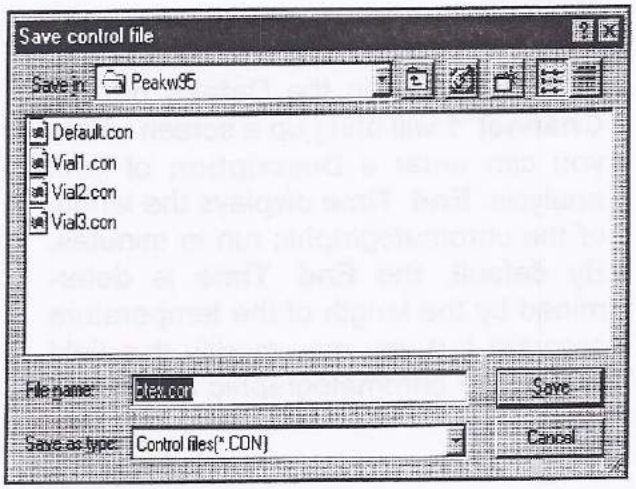


PeakSimple for Windows uses **Control Files**, identified with the **.CON** extension, to save the operating settings of specific methods. To load a **Control File**, drop down the **FILE** menu and select **OPEN CONTROL FILE**. A window will open which will allow you to use standard Windows navigating tools to select from a list of **.CON** files, located on the **Drive** or **Directory** of your choice. Click on the desired **File Name** and then click **O.K.**

The FILE-SAVE CONTROL FILE Pull-Down Menu



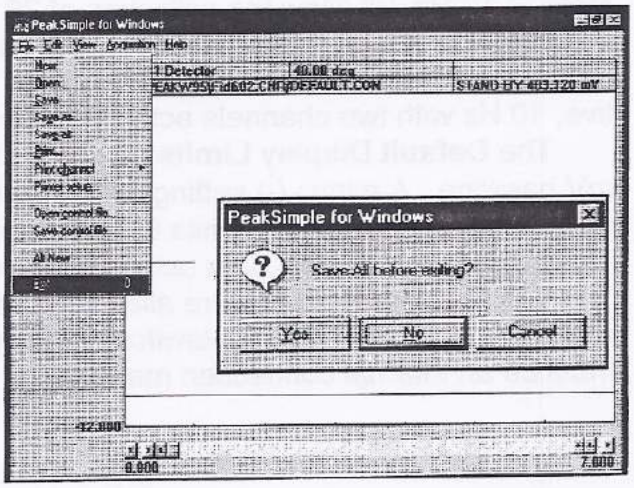
Once you have set up all of the user-definable parameters within PeakSimple for Windows that meet the requirements of your system and/or your specific analytical method, it is wise to save these settings for future use. PeakSimple uses **control files**, identified with a **.CON** extension, to save the operating settings of specific methods, this includes the event table, temperature program, component table, print information, calibration table, etc.



A **control file** is like a photocopy of your operating settings that you can reload for use at any time. When using **control files**, you only need to set analysis parameters once and then save them using a descriptive filename, followed by the **.CON** extension, (for example, **BTEX.CON**). To save the **control file**, drop down the **File** menu and select **Save control file**. Enter the name for your file in the **File name** box and click **O.K.**. If you want these current settings to be loaded by default each time you start PeakSimple, name the control file **Default.con**.

FILE-ALT NEW

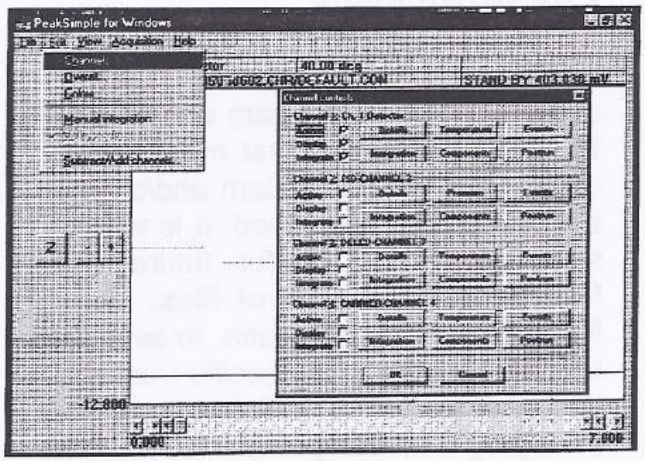
The **FILE-ALT NEW** feature will clear the display of all active channels in the **Alt**ernate timebase without starting a new chromatographic run.



FILE-EXIT

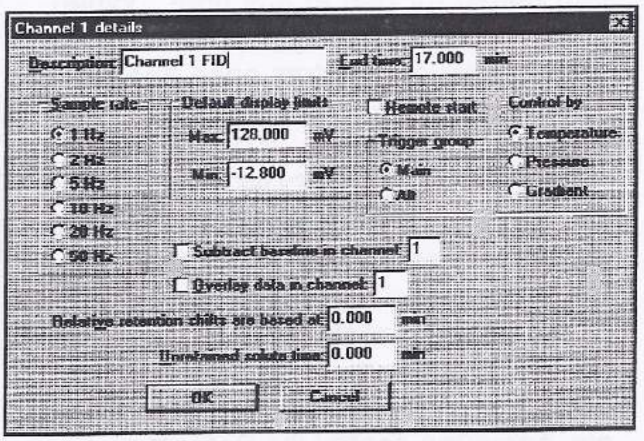
Exits PeakSimple for Windows. Click **Yes** to save any changes made to your **control file** parameters.

The EDIT-CHANNELS Pull-Down Menu



The **EDIT** pull-down menu allows you to modify most of the operating parameters for your specific application. Selecting **EDIT-CHANNELS** will bring up a screen which will enable you to select which of the four channels are **active, displayed and integrated**. Each channels' operating parameters such as **Details, Temperature, Events, Integration, Components and Postrun** information can be easily modified.

The EDIT-CHANNELS-DETAILS Screen



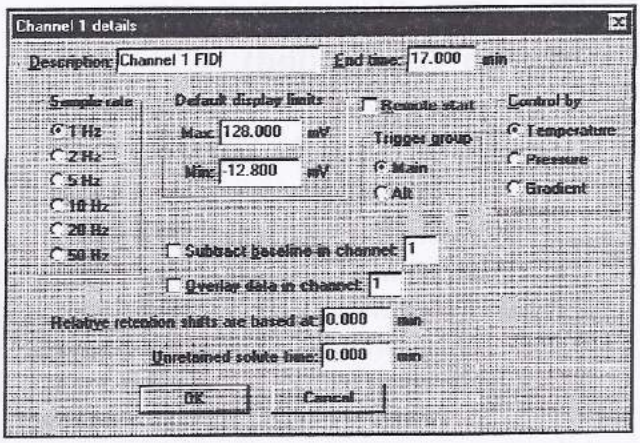
Clicking on the **Details** box for **Channel 1** will bring up a screen where you can enter a **Description** of your analysis. **End Time** displays the length of the chromatographic run in minutes. By default, the **End Time** is determined by the length of the temperature program but you may modify this field to end the chromatographic run at any time.

The **Sample Rate** should be set to a rate sufficient to ensure that 20 data samples are collected for each peak. For example: A **Sample Rate** of 1 Hz will allow the collection of 20 data points from a peak 20 seconds wide from base to base. And a **Sample Rate** of 10 Hz will allow the collection of 20 data points from a peak 2 seconds wide from base to base. The analog to digital converter is limited in its ability to sample high rates when many channels are active. The limits are: 50 Hz with one channel active, 10 Hz with two channels active and 5 Hz with three or four channels active.

The **Default Display Limits** can be adjusted to view data above and below the 0 mV baseline. A minus (-) setting for **minimum** will display negative going peaks. The ratio of **min./max.** display limits is maintained when you click on the Display minus and plus buttons in the main data acquisition screen.

The **Remote Start** feature allows the user to start a chromatographic run using an external signal such as a footswitch. Check the box to enable **Remote Start.** (There must be an internal connection made to the A/D board in order for this option to work.)

The EDIT-CHANNELS-DETAILS Screen (continued)



Trigger Group

The **Trigger Group** selection assigns the channel to the **Main** or **Alt** trigger group. The picture at right shows the **Channel 1 Details** screen with the **Main Trigger Group** selected.

Any **Channel** with the **Main** trigger group selected will start running when the SPACEBAR is pressed and end when the END key is pressed. Any **Channel** with the **Alt** trigger group selected will start running when the + (plus) key is pressed and end when the – (minus) key is pressed. When acquiring four detector signal inputs from one gas chromatograph; verify that all four channels' **Trigger Group** is set to **Main**. This ensures that all four channels are acquiring data synchronously by using the same timebase. If two channels of data are coming from an SRI gas chromatograph, and you also wish to acquire two channels from an external input device such as an HPLC, then select the **Alt** trigger group for channels 3 and 4. This allows for asynchronous data collection.

Subtract Baseline In Channel "X"

Checking **Channel 1's** box for **Subtract Baseline In Channel "X"**, where **"X"** is 1,2,3 or 4, will cause the chromatogram in **Channel 1** to subtract the baseline stored in **Channel "X"**, while running in real-time. Load the baseline to be subtracted into an inactive channel to ensure that the data is not deleted by the start of a new run on that channel. (Uncheck the **active** box, see **Edit-Channels**). Baseline subtraction can also be performed using PeakSimple's **Edit-Subtract/Add Channels** feature, however, this is not a real-time function, but a post-run function, done at the end of the chromatographic run.

Overlay Data In Channel "X"

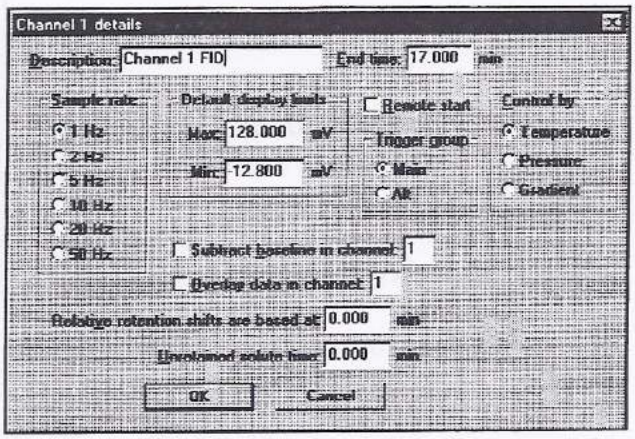
Checking **Channel 1's** box for **Overlay Data In Channel "X"**, where **"X"** is 1,2,3 or 4, will overlay the data stored on **Channel "X"** onto **Channel 1** using contrasting colors. The channel selected for overlay can be either an active or inactive channel. When the overlay channel is active then the overlay will be seen in real-time.

Relative Retention Shifts Are Based At "X" Minutes

Relative Retention Shifts Are Based At "X" Minutes. Enter into this box the time, in minutes, that the sample is actually injected onto the column. This is done to ensure that relative retention times are correctly calculated. See the **EDIT-CHANNEL-COMPONENTS** section of this manual for more details.

The EDIT-CHANNELS-DETAILS Screen (continued)

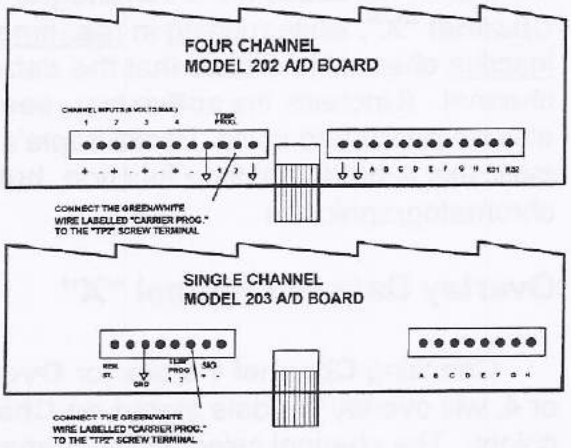
Unretained Solute Time



If resolution has been selected to be printed in the chromatogram report, then a **Unretained Solute Time** value needs to be entered to ensure correct resolution calculations. Enter the number of minutes an **Unretained Solute** takes to pass through the column. This value is used in the determination of peak resolution statistics.

Control By

The A/D Board that is built into the SRI gas chromatograph includes two digital-to-analog converters or DACs. DAC1 is primarily used to control the column oven #1 **temperature** ramp by introducing 10mV / °C to the oven heating circuit and is programmable by editing the **Channel 1–Temperature** control window. DAC2 is primarily used to control the column oven #2 **temperature** ramp. Carrier gas E.P.C. pressure is also programmable by editing the **Channel 2–Temperature/Pressure** control window. The DACs may be used to control **Pressure** by following the procedure described below and then selecting **Pressure** in the **Control By** window of the **Edit-Channels-Details** screen.



To avoid startup difficulties, the Carrier E.P.C. is shipped disabled. To enable the use of the DACs to set up a **Pressure Program**, only a single wire needs to be moved inside the G.C.. Unplug the G.C. and remove the six screws which secure the bottom cover. Tilt the G.C. onto its back and remove the bottom cover. The A/D Board is green in color and is mounted on the right-hand side of the G.C. chassis. Locate the Green wire with a White stripe on the A/D Board. This is the **Carrier Program** wire. Normally this wire is connected to a ground (GD) screw terminal. Unscrew the **Carrier Program** wire and connect it to the temperature/pressure #2 (TP2) screw terminal also on the A/D Board. Re-attach the bottom cover, connect power and re-establish communication between the G.C. and the computer. Select **Pressure** in the **Control By** window of the **Edit-Channels-Channel 2-Details** screen. A pressure program ramp set up in **Channel 2** will now control the Carrier Gas E.P.C. pressure by introducing 10mV for every P.S.I.. Turn the Carrier 1 **Local Setpoint** to zero. This is necessary since the Local setpoint is added to the programmed E.P.C. input in determining the Carrier 1 **total setpoint**.

The EDIT-CHANNELS-DETAILS Screen (continued)

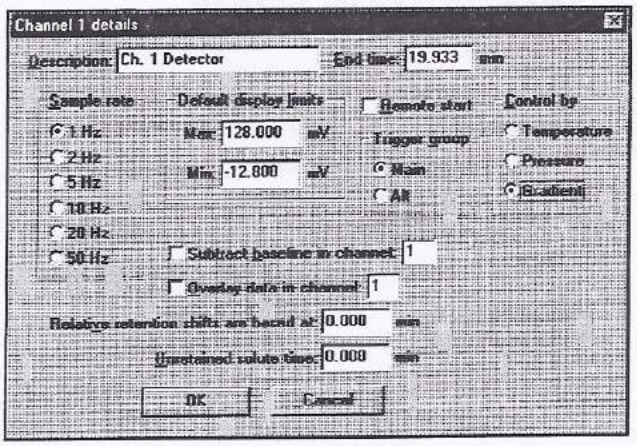
Setting Up Gradients for Liquid Chromatography

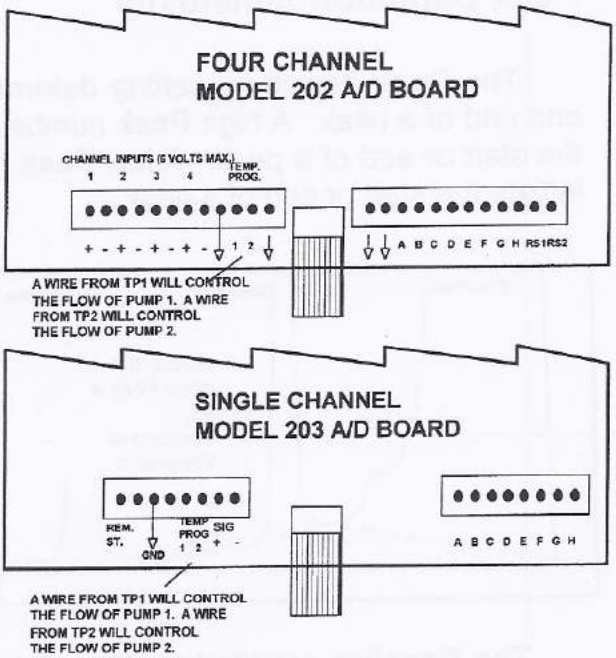
Data System users may wish to use the A/D Board DACs for setting up an HPLC solvent gradient. PeakSimple for Windows allows the user to control the flow of two pumps, provided they operate from a zero to five volt (0-5V) ramp input.

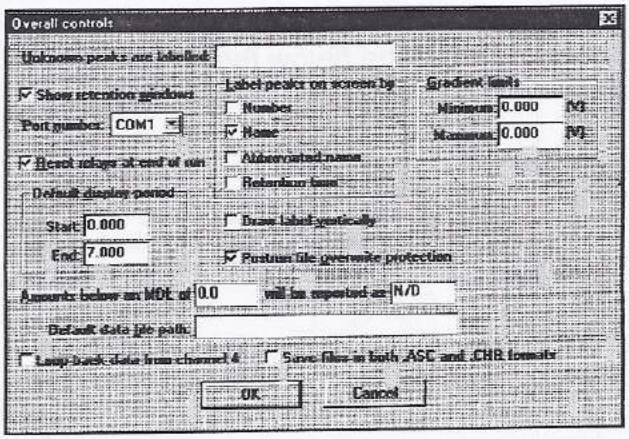
To operate the pumps, several internal connections must be made between the HPLC and the Data System. Unplug the Data System and remove the two screws which secure the top cover. Route the Pump A and Pump B control wires from the HPLC to the Data System and connect the Pump A control wire to TP1 and the Pump B control wire to TP2. Re-attach the top cover, connect power and re-establish communication between the Data System and the computer.

Set up the **Gradient** ramp on **channel one** (TP1) to control the flow of Pump A into the system (10mV / %) and the **Gradient** ramp on **channel two** (TP2) to control the flow of Pump B. Modifying the **Gradient** ramp program on **Channel 1** to rise from 10% to 90% will automatically create a **Gradient** ramp program on **Channel 2** that decreases proportionately from 90% to 10%.

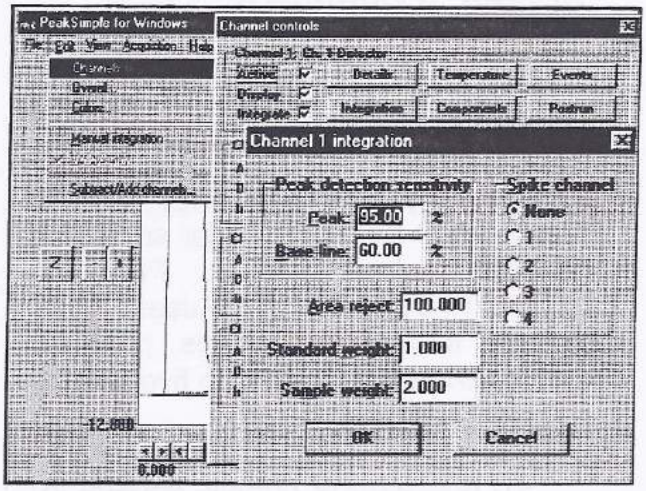
Gradient Limits Zero and **Span** may be scaled in the **Edit-Overall** screen to account for any offsets. PeakSimple allows for a voltage offset and scaling factor in these fields to calibrate the voltage output to match the pump's requirements.







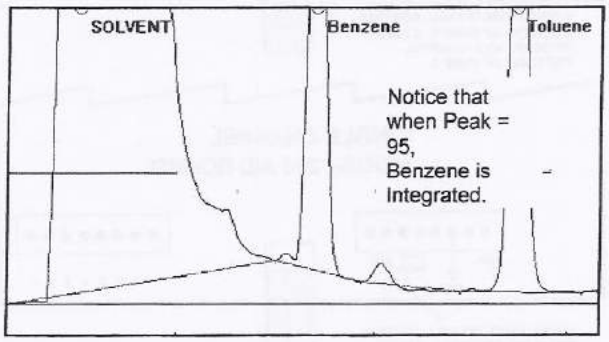
The EDIT-CHANNELS-INTEGRATION Screen

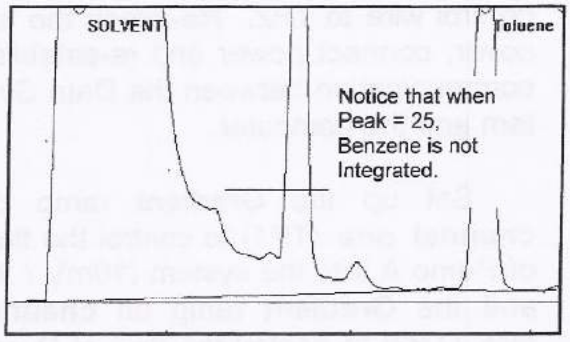


PeakSimple for Windows allows you to define specific integration parameters necessary for the proper analysis of your sample data, such as peak and baseline sensitivity and area reject. Any of the **Integration** parameters described below may be modified either before or after data collection. Pressing the **ENTER** key will update the report and the results of the chromatogram currently being displayed.

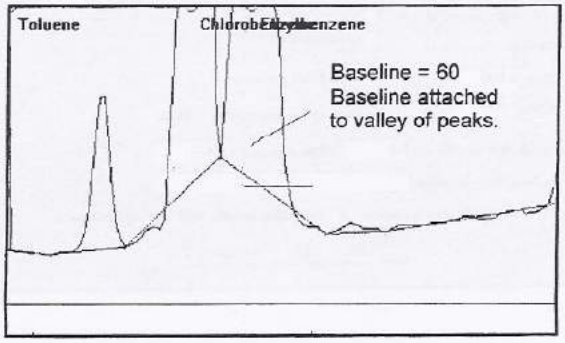
Peak Detection Sensitivity

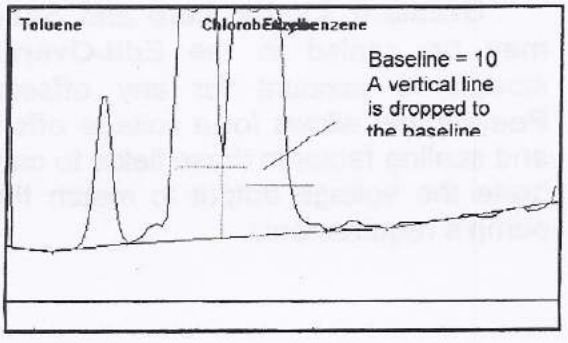
The **Peak** sensitivity setting determines how PeakSimple detects the beginning and end of a peak. A high **Peak** number requires only a small slope change to initiate the start or end of a peak. A low **Peak** number requires a very large slope change to initiate the start or end of a peak.





The **Baseline** sensitivity setting determines how PeakSimple attaches the baseline to the data line. The larger the **Baseline** number; the more likely PeakSimple will draw the baseline to a valley between two peaks. The smaller the **Baseline** number; the more likely PeakSimple will drop a vertical line from a valley to a horizontally constructed baseline below the peak.





The EDIT-CHANNELS-INTEGRATION Screen (continued)

Area Reject

If a chromatogram contains peaks whose area counts fall below the threshold defined by the **Area Reject** for that channel, the peak will be ignored and no integration will occur. If the peak area is of interest, you can lower the **Area Reject** value until the peak in question is integrated. Integrated peaks are marked with a circle at the top of the peak.

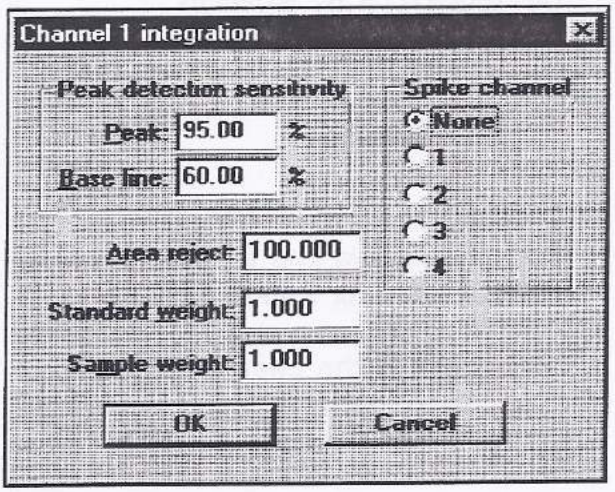
Standard Weight

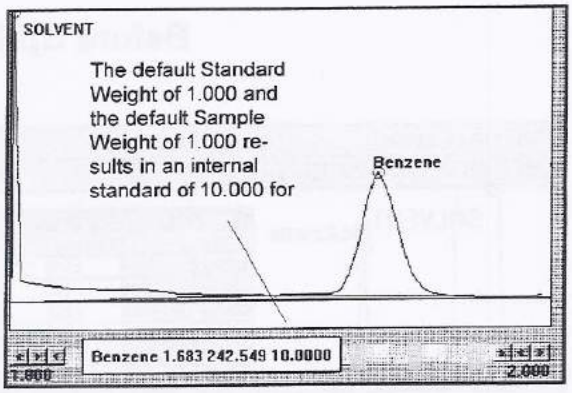
PeakSimple for Windows determines the internal or external standard results by the ratio of the STANDARD divided by the SAMPLE.

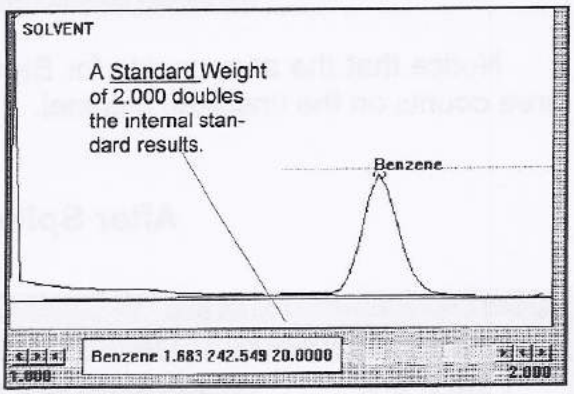
The **Standard Weight** setting may be changed to adjust the channel's quantification, affecting internal or external peak results by the factor entered. For instance: A setting of 2.000 will double the weight of the standard thereby doubling the internal or external standard results. (Increased to 20.000 in the example shown.)

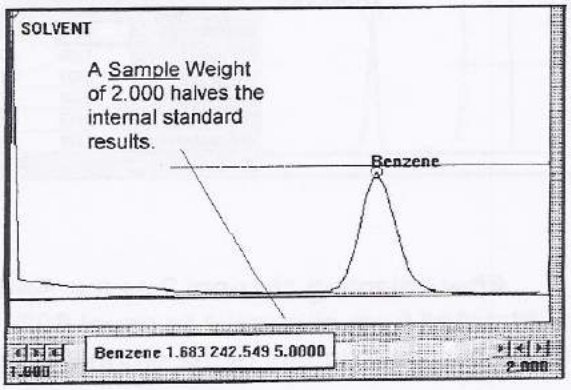
Sample Weight

The **Sample Weight** setting may also be changed to adjust the channel's quantification, affecting internal or external peak results by the factor entered. For instance: A setting of 2.000 will double the weight of the sample thereby halving the internal or external standard results. (Decreased to 5.000 in the example shown.)

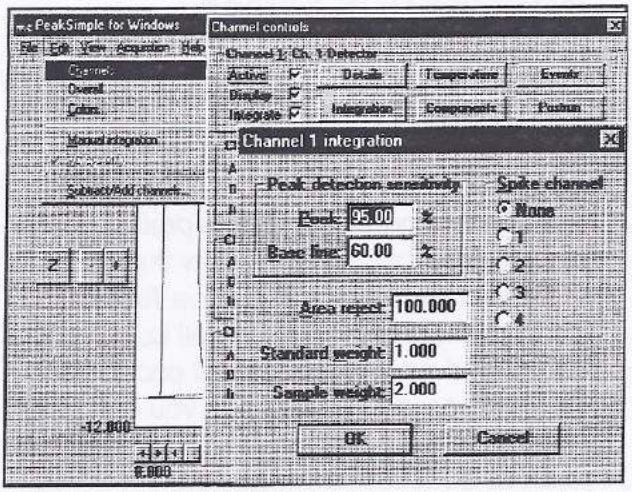








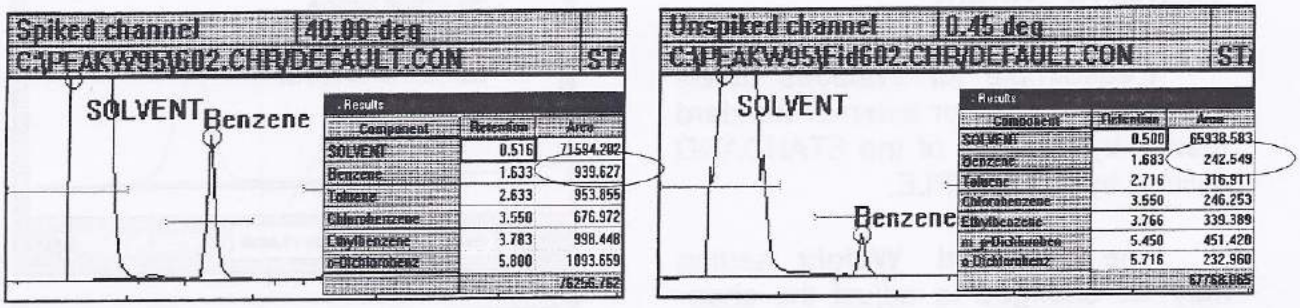
The EDIT-CHANNELS-INTEGRATION Screen (continued)



Spike Channel

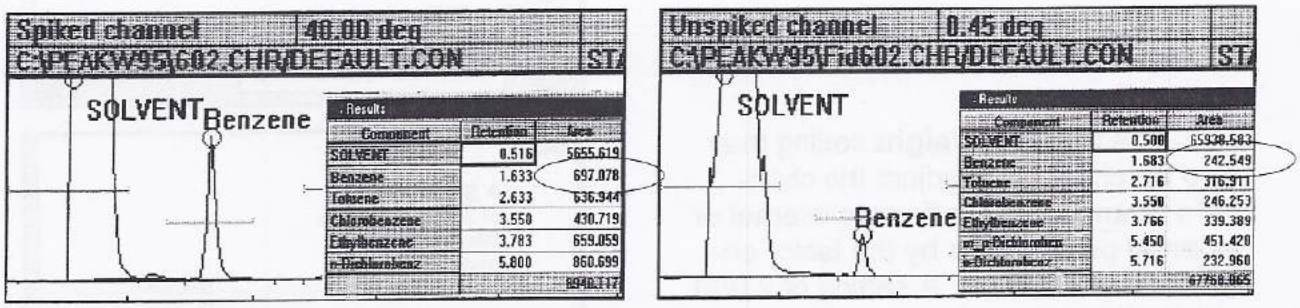
Another feature of PeakSimple for Windows allows you to display the results of a matrix **Spike Channel** subtraction. The example shown below demonstrates the peak area counts of a unspiked channel being subtracted from the area counts of a spiked channel.

Before Spike Channel Subtraction



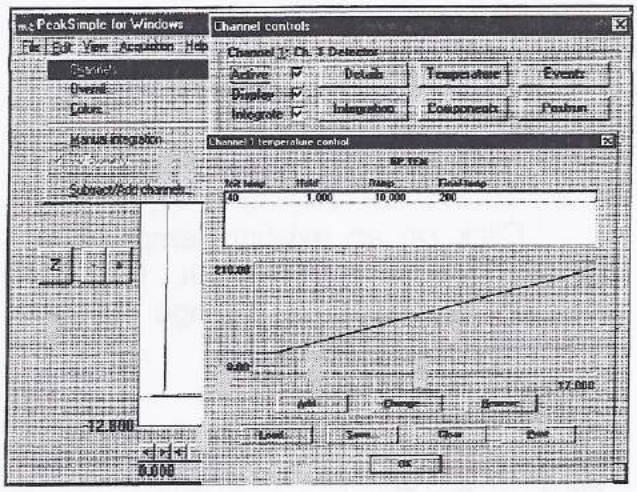
Notice that the area counts for Benzene are 939 on the spiked channel, and 242 area counts on the unspiked channel.

After Spike Channel Subtraction



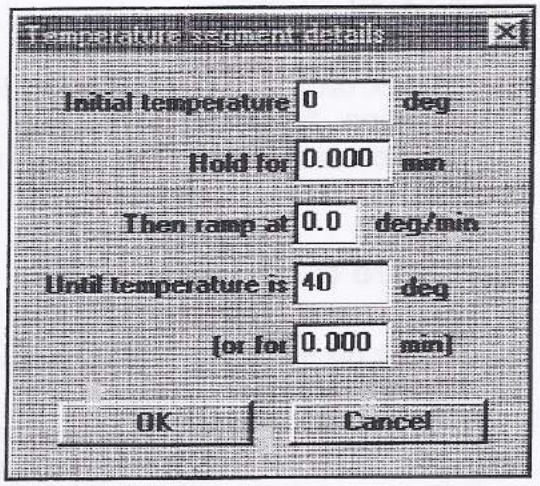
After selecting channel 2 as the **Spike Channel**, the area counts for channel 2 are subtracted from channel 1 to equal 697, (939 – 242 = 697). The difference of 697 indicates the area counts of the amount of sample spiked into channel 1.

The EDIT-CHANNELS-TEMPERATURE Screen



PeakSimple for Windows features temperature-programming of the G.C 's column oven(s). Access the **Edit-Channel 1-Temperature screen** to specify the temperature parameters to be used during the analytical run. The temperature program is capable of executing an unlimited number of temperature ramp and hold periods during the analysis as well as maintaining a single temperature throughout the run for isothermal operation.

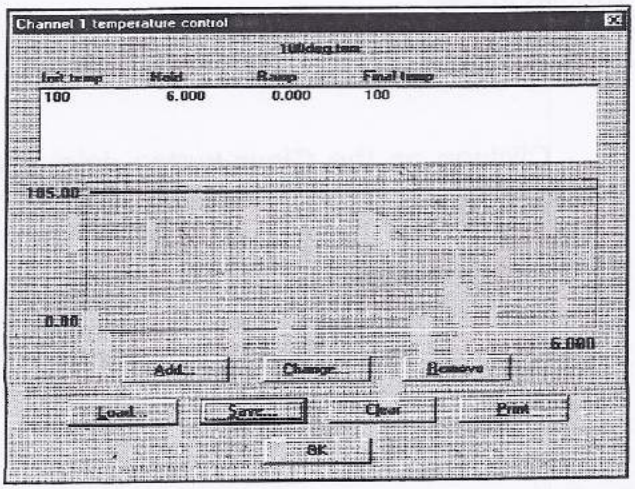
The Temperature Segment Details Screen



The **Add** Button

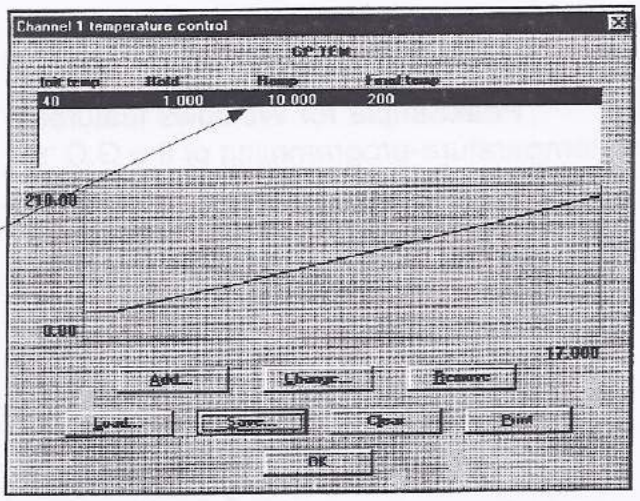
Click on the **Add** button from a blank **Channel 1 temperature control** window to create a new temperature program for Column oven #1. (Use the **Edit-Channel 2-Temperature** screen for controlling column oven #2). Type in the required data in the following fields; **Initial temperature**, the **Hold** period in minutes, the **Ramp** rate in °C / min, and the final **Temperature**, or the duration of the Ramp.

The length of the run is automatically calculated by PeakSimple based on the information provided in these fields, and is also displayed in the **Edit-Channels-Details End Time** field. Additional ramp segments may be added by clicking the **Add** button again.



In isothermal operation, the **Initial** and the final temperature are the same, so a **Ramp** rate of 0.000 is entered. The **Hold** period determines the length of the analytical run.

The EDIT-CHANNELS-TEMPERATURE Screen (continued)

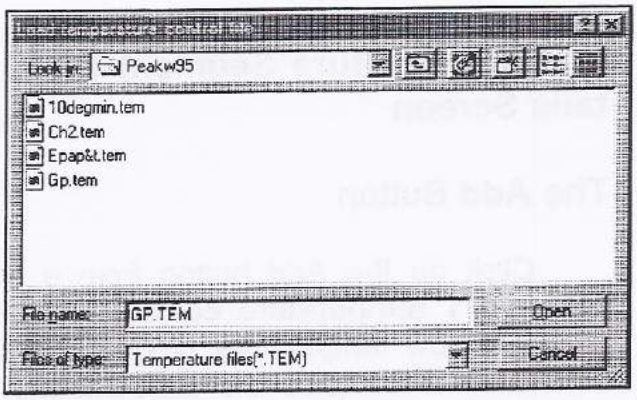


The **Change** Button

Click on an existing temperature program segment to select it. Click on the **Change** button to change the parameters of the segment.

The **Remove** Button

Click on the **Remove** button to remove the segment from the current program.

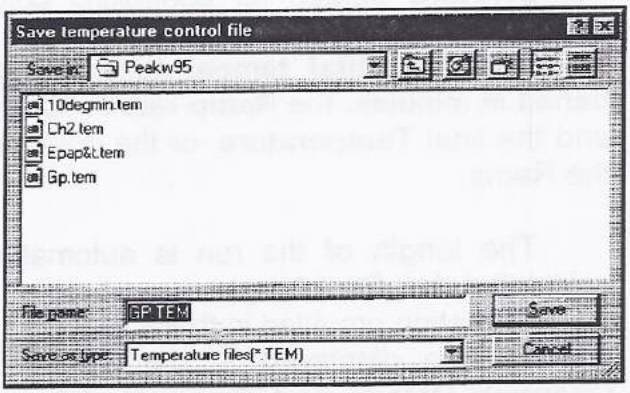


The **Load** Button

Click on the **Load** button to load an existing temperature control file, designated with the **.TEM** file extension.

The **Save** Button

Click on the **Save** button to save a new temperature control file, or to update an existing one. Remember to use the **.TEM** extension when naming the temperature control file. The saved file name appears at the top of the temperature control window indicating the file in use.



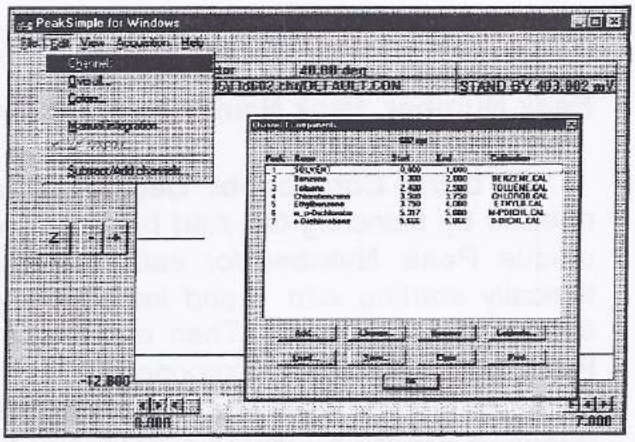
The **Clear** Button

Clicking on the **Clear** button deletes all temperature data from the temperature control window. The temperature program name is also removed.

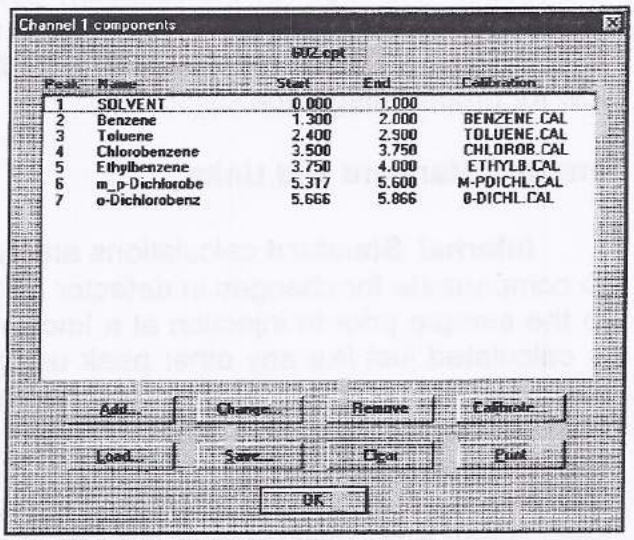
The **Print** Button

Clicking on the **Print** button sends the file data and temperature program profile to the printer.

The EDIT-CHANNELS-COMPONENTS Screen

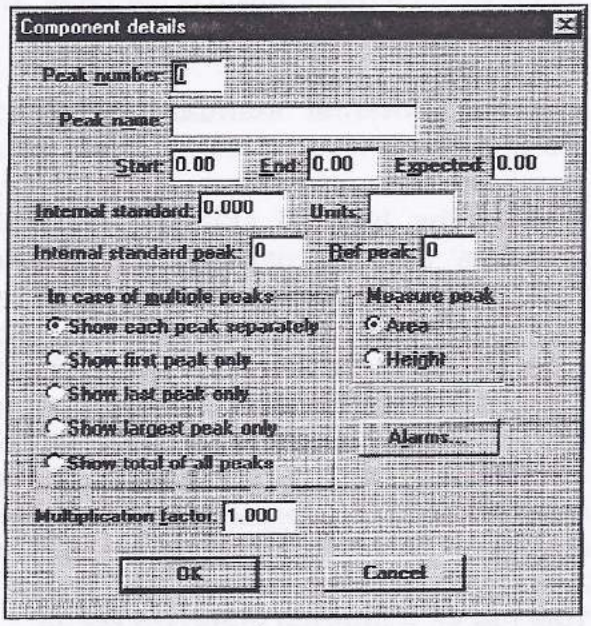


PeakSimple for Windows can identify and quantify sample components through the use of a component table. The component table enables PeakSimple to recognize each peak by its retention time and compare the area counts against the calibration curve to produce actual concentration data. The user can edit the component table for each channel by accessing the **Edit-Channels-Components** screen.



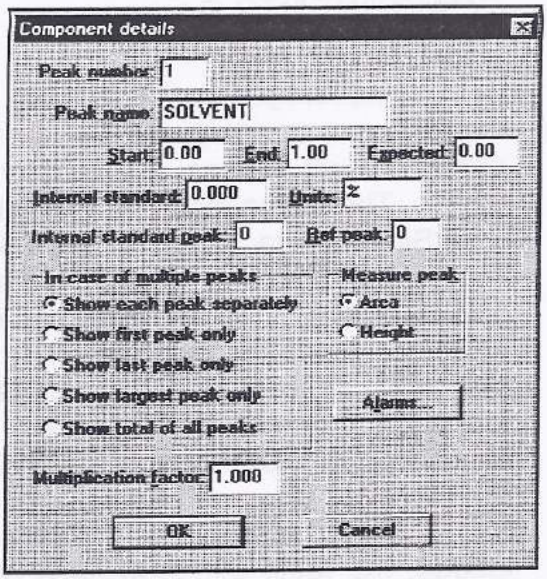
When a component table is loaded, the table will show each component by its peak number, peak name, the start time for the retention window, the stop time for the retention window, and the associated calibration file name. Different component tables may be used for each active channel and any component table can be saved as a component file for future use. Component files are designated with a **.CPT** extension. The component file-name appears at the top of the **Components** screen.

COMPONENT DETAILS



Select **Add** to add a new component to a blank or existing component table. The Component Details screen will open allowing the user to input specific peak parameters. As a minimum, enter the **Peak Number**, **Peak Name**, **Start** time and **End** time. Other optional parameters are the **Expected** peak time, the concentration **Units** to be reported, any **Internal Standard** or **Reference** peak information, peaks measured by **Area** or **Height**, handling of **Multiple Peaks**, the **Multiplication Factor** and **Alarm** parameters.

The EDIT-CHANNELS-COMPONENTS-DETAILS Screen (continued)



Peak Number, Peak Name, Start and End

A blank **Component Details** screen is opened by selecting the **Add** button. Enter a unique **Peak Number** for each component, typically starting with **1** and incrementing for each additional peak. Then enter a unique **Peak Name** for each component. **Start** and **End** define the beginning and ending of the retention windows, which is used to identify the peak. The width of the retention window should be set wide enough so that small fluctuations in the peak's retention time will still allow for proper integration.

Internal Standard and Units

Internal Standard calculations are used to correct for injection size variations, or to compensate for changes in detector sensitivity. An internal standard peak is added to the sample prior to injection at a known concentration. The internal standard peak is calculated just like any other peak using a calibration curve, typically a single point calibration. The known concentration of the internal standard peak is entered into the **Internal Standard** dialog box of the **Component Details** screen. In the example shown below, Benzene has been chosen as the internal standard peak. The known concentration of Benzene is entered as **100**, and **ppm** is entered in the **Units** dialog box. When a chromatogram is integrated and a report is produced, the external calculation yields a result which is the **peak area x calibration factor** (slope of the calibration curve) **= external standard result**.

The **internal standard** calculation yields a result which is the **external result times the ratio of the known concentration of the internal standard peak divided by the external result for the internal standard peak**. As shown in the example to the right, note that while the external result for Benzene yields 104.95, the internal result yields exactly 100 (the known concentration) as a result of the calculation **104.95 x 100/104.95**. In the same way, the internal result for every analyte peak which is referenced to Benzene is calculated as **external result x 100/104.95 = internal standard result**.