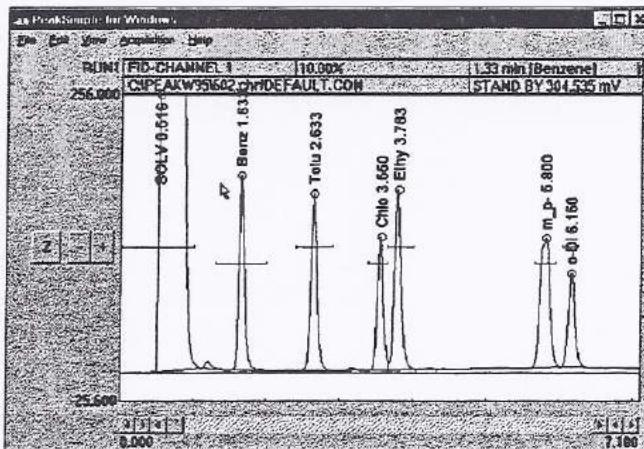


# PeakSimple for Windows Software and Chromatography Data System Validation Statement



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 acquisition 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.

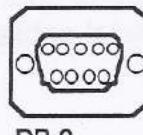
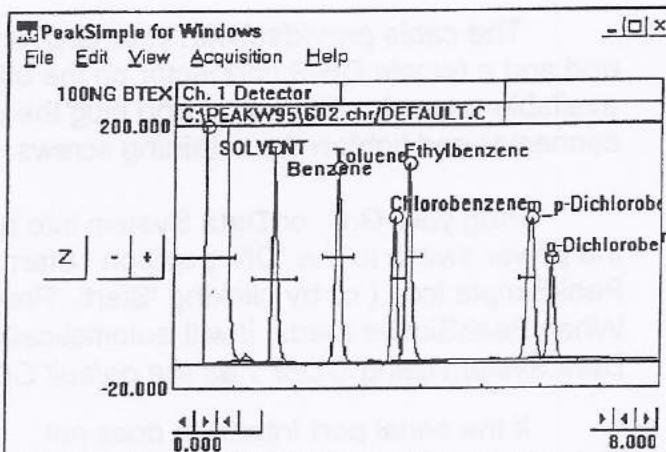
The earlier IBM PC-compatible ISA expansion bus data acquisition cards (AD100 and AD110) used by PeakSimple II and PeakSimple III data systems are *not supported* by PeakSimple for Windows. However, all chromatograms acquired using DOS-based PeakSimple II and PeakSimple III continue to be compatible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

### Identifying Your COM Port

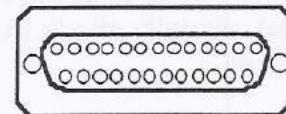
Before attempting to establish communication between your G.C. and the serial data system interface, be sure to check that all the necessary electrical connections have been made, including the connection of any optional remote start cables.

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

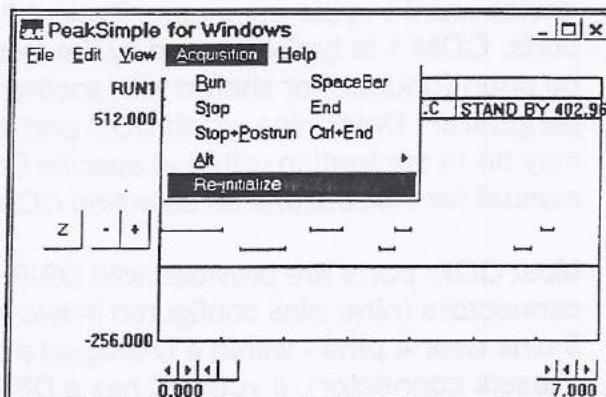
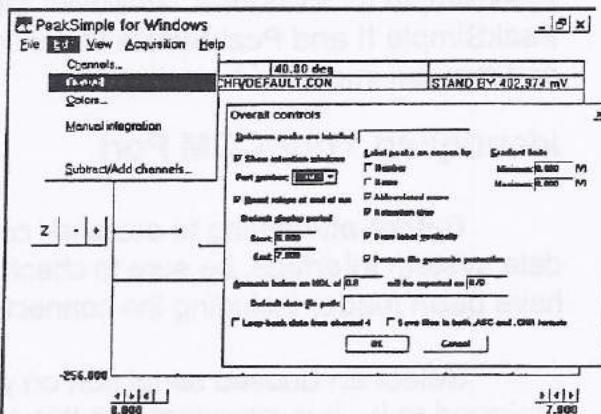
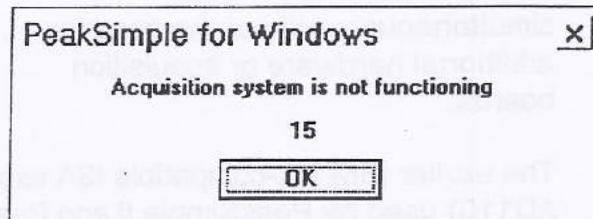
The cable provided with your G.C. or data system has a male DB-9 plug on one end and a female DB-9 connector on the other end. Plug one end of this cable into your available computer COM port and plug the other end into the G.C. or Data System DB-9 connector and tighten the retaining screws.

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

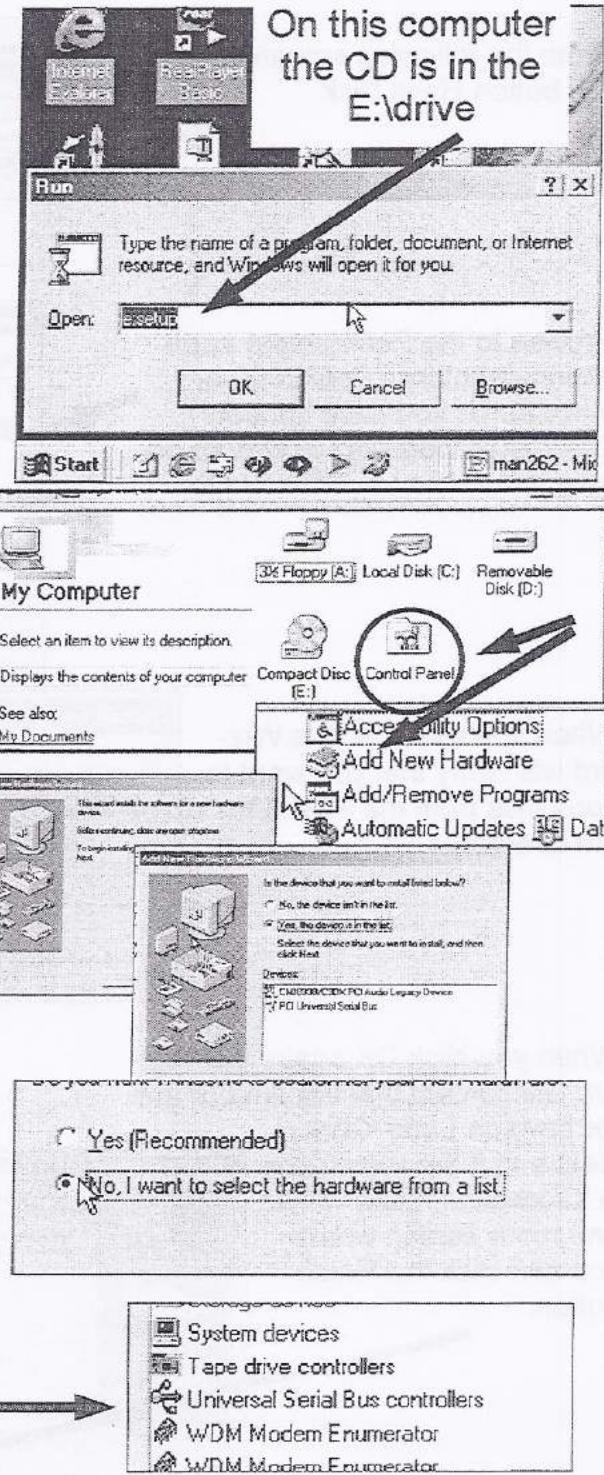
Install PeakSimple software from the installation CD or from a download from SRI's website <http://www.srigc.com>. The download is a zip file which must be un-zipped using PKZip or WinZip. From the Windows RUN command click on setup.exe in either the CD drive or the directory where the download was saved.

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.

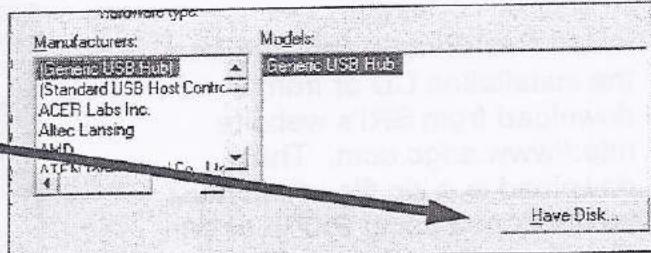
Scroll down the list until you can click on Universal Serial Bus controllers



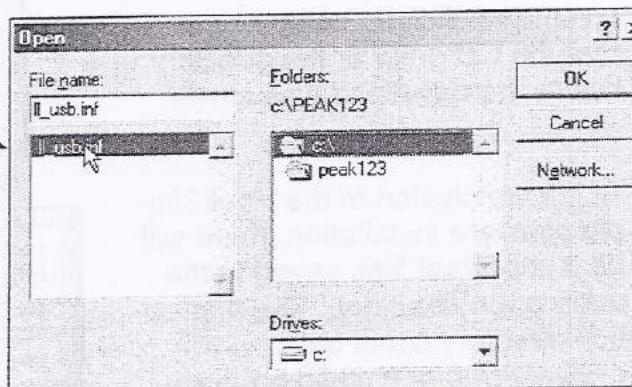
## Chapter: PeakSimple

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

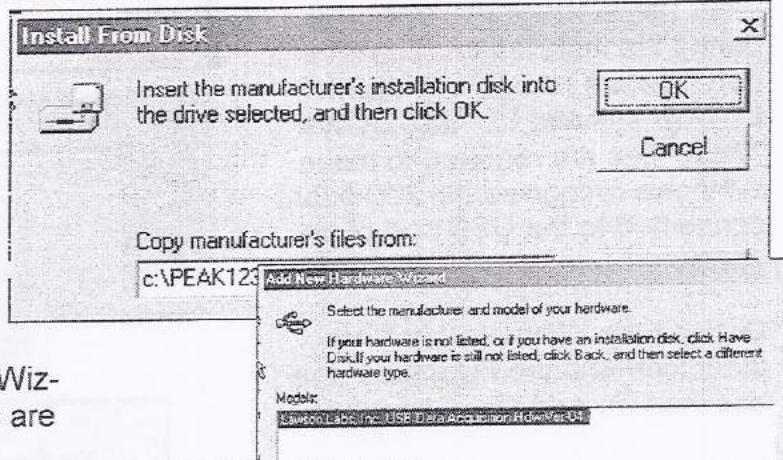
From the following screen click on the button Have Disk



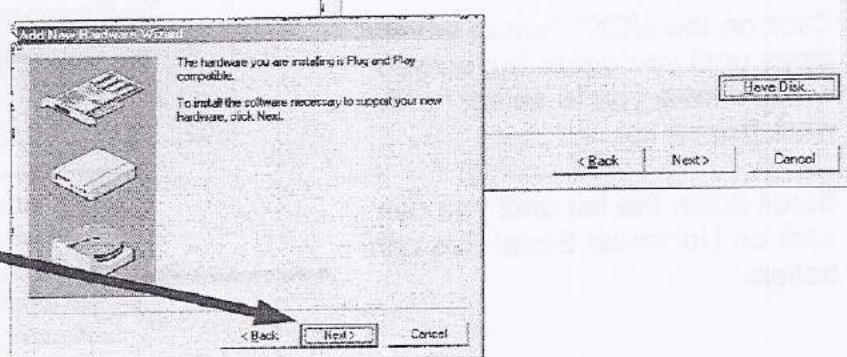
Browse to the PeakSimple application directory ( Peak2000 or other name you have chosen ). The Installation Wizard should be able to find the LL\_USB.inf file.



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.

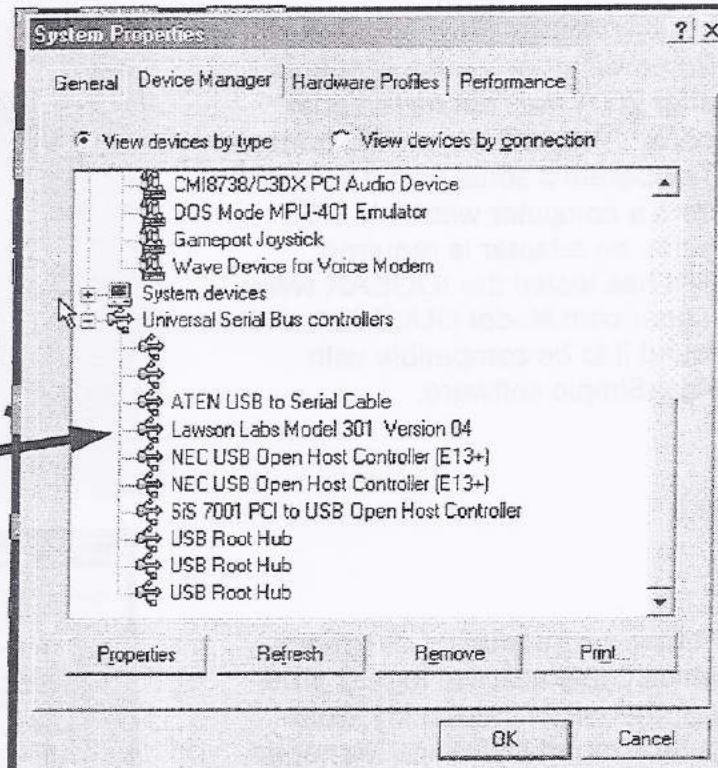


## Chapter: PeakSimple

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

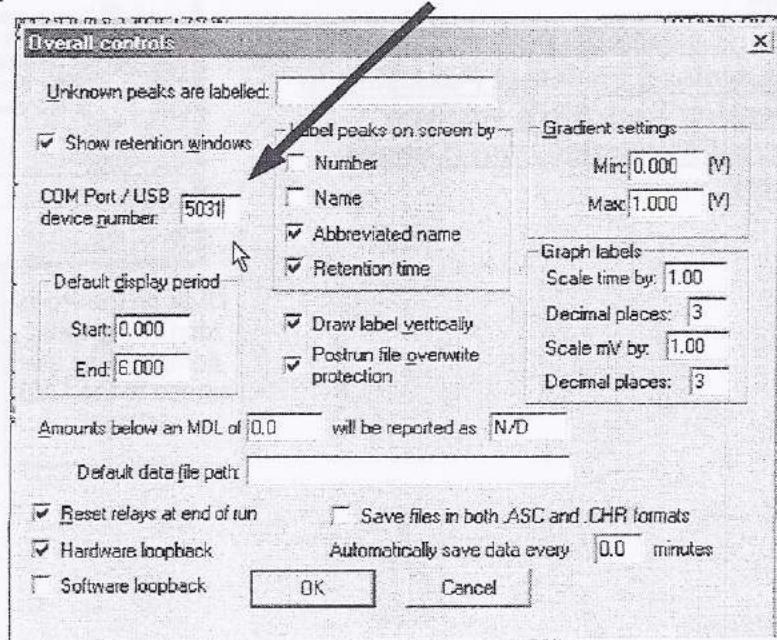
You must RESTART the COMPUTER before the drivers will work.

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

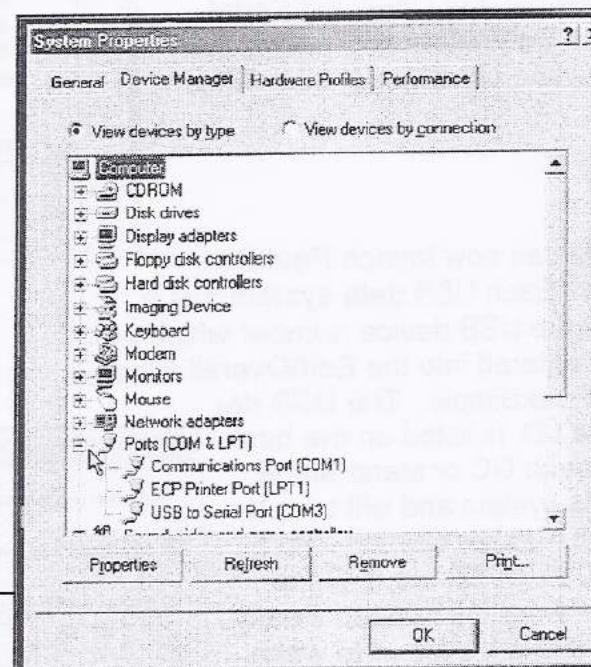
Topic: Operation of serial port Models 203 and 202 on computers with USB ports only

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).

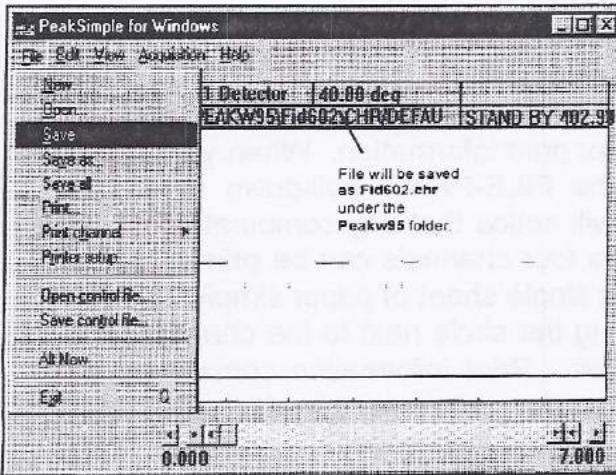
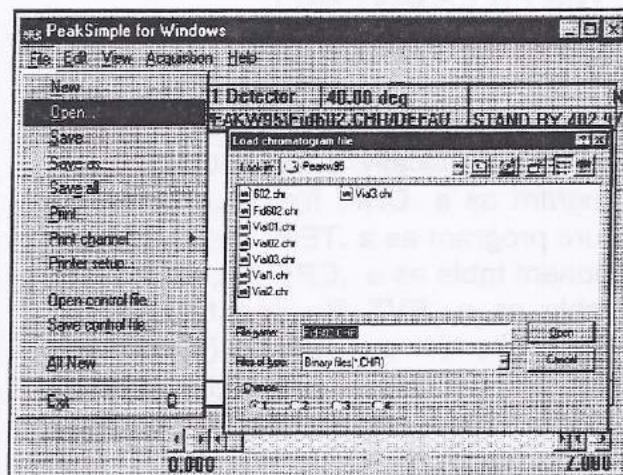
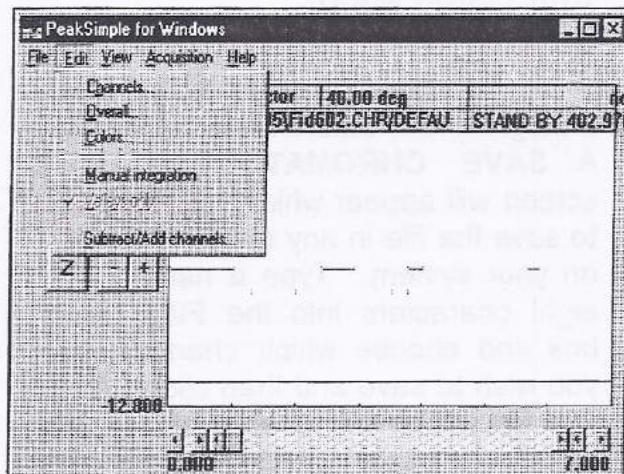
### The FILE Pull-Down Menu

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 then 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

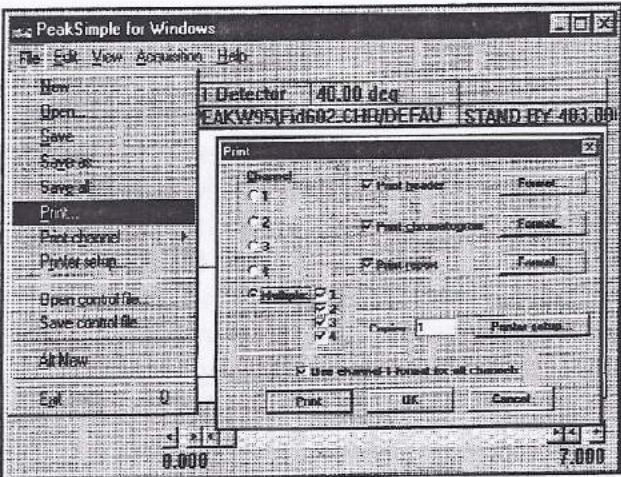
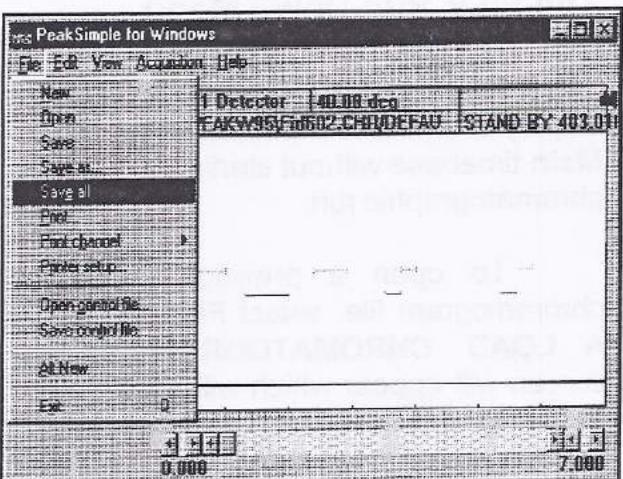
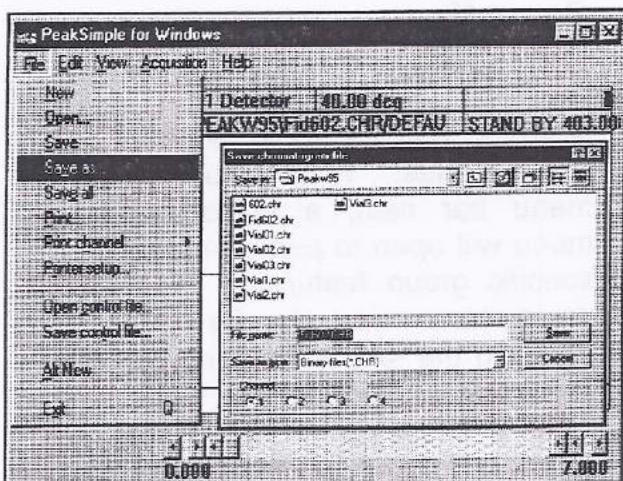
To save a newly created chromatogram file, select **FILE-SAVE AS**. A **SAVE CHROMATOGRAM FILE** screen will appear which will allow you to save the file in any directory (folder) on your system. Type a name up to eight characters into the File Name box and choose which channel (1-4) you wish to save and then 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 **AS-CII** 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.



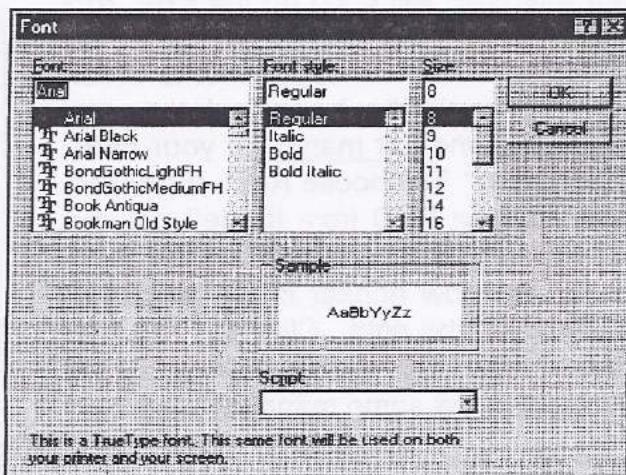
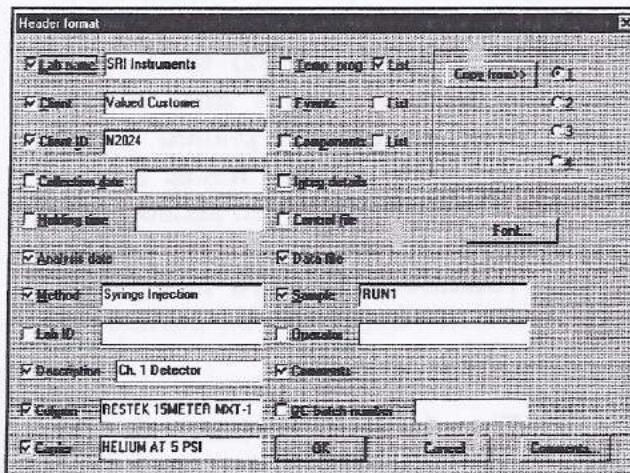
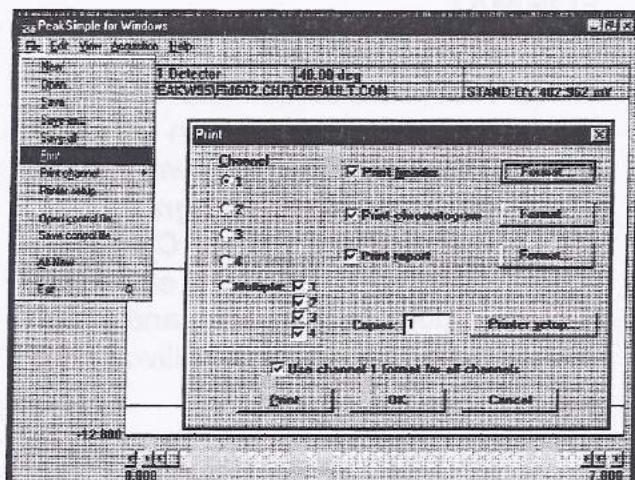
## The FILE-PRINT Pull-Down Menu (CHANNEL 1)

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.

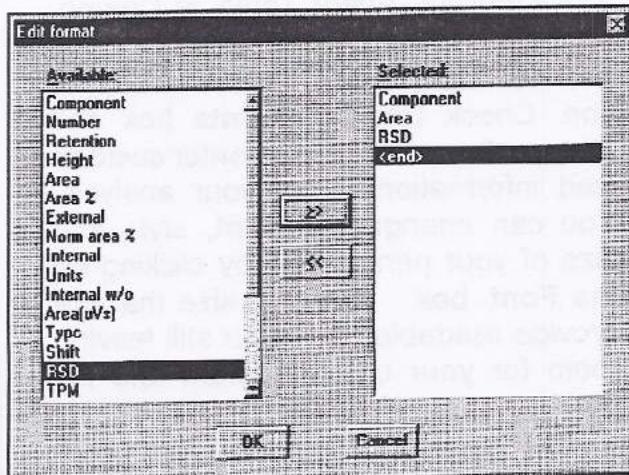
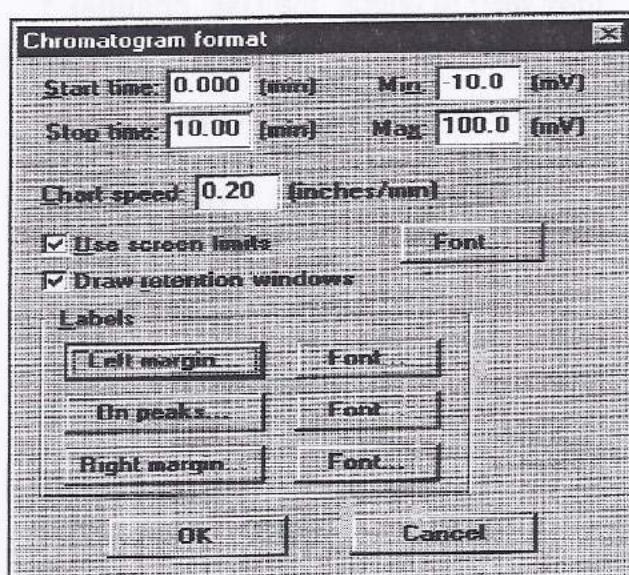
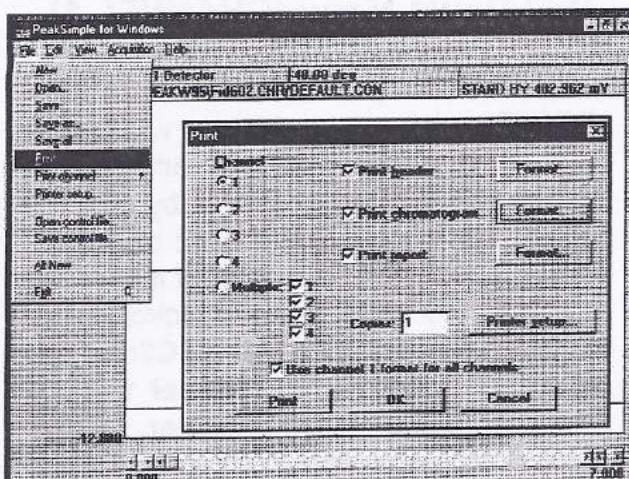


## PRINT CHROMATOGRAM FORMAT

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.



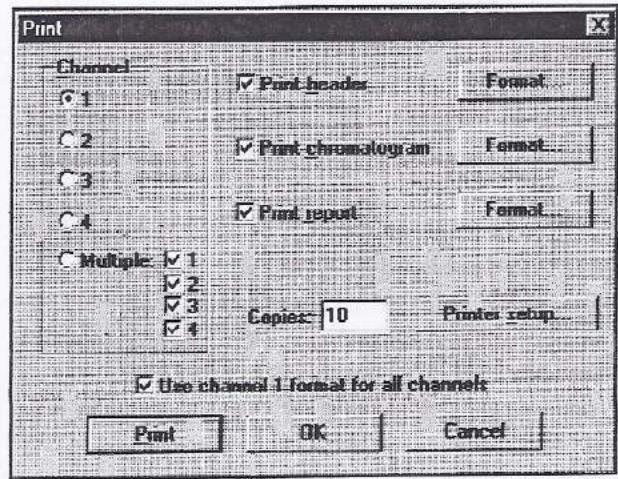
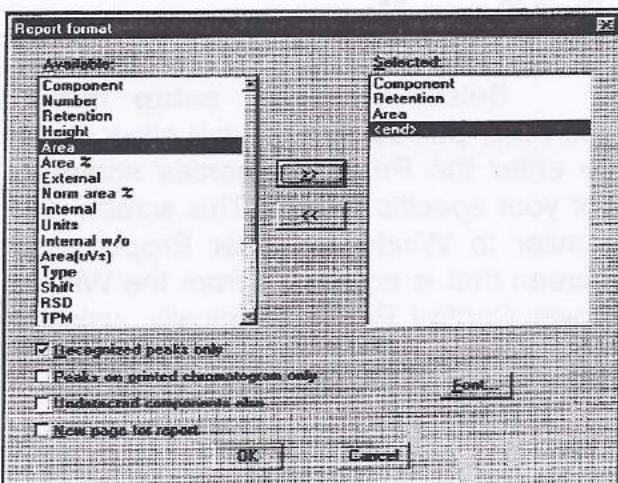
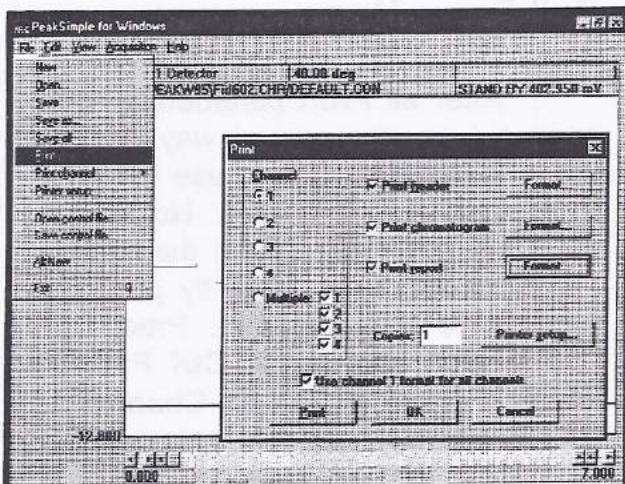
## PRINT REPORT FORMAT

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.

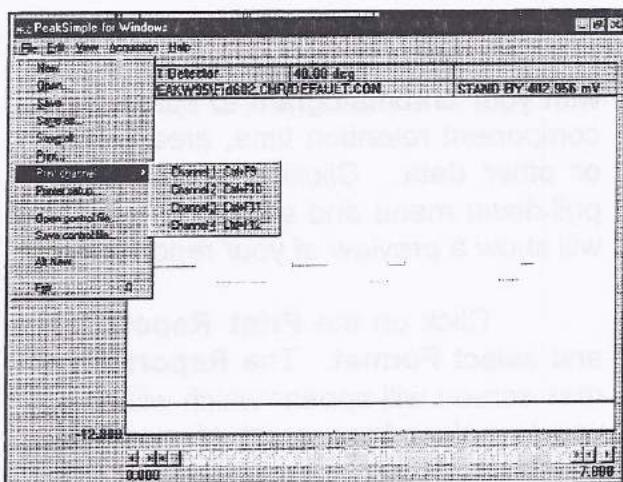
Clicking on the box next to **Recognized peaks only** will place a check mark in the box and only those peaks which integrate properly within named retention windows will be printed in the report. Checking the **Peaks on printed chromatogram only** box will allow the report to show only those peaks defined 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**.



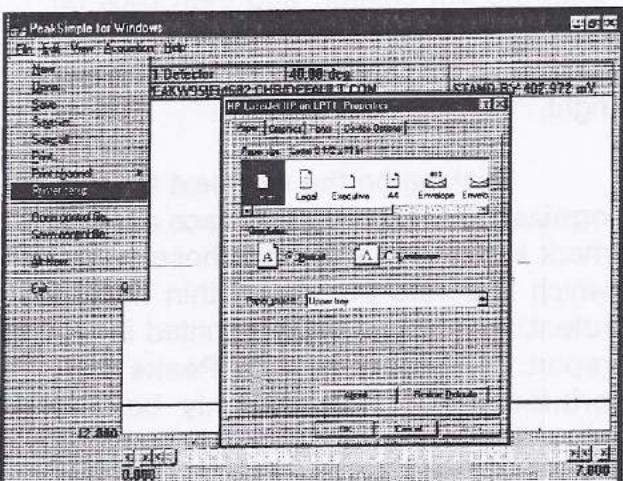
## The FILE-PRINT CHANNEL Pull-Down Menu

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.



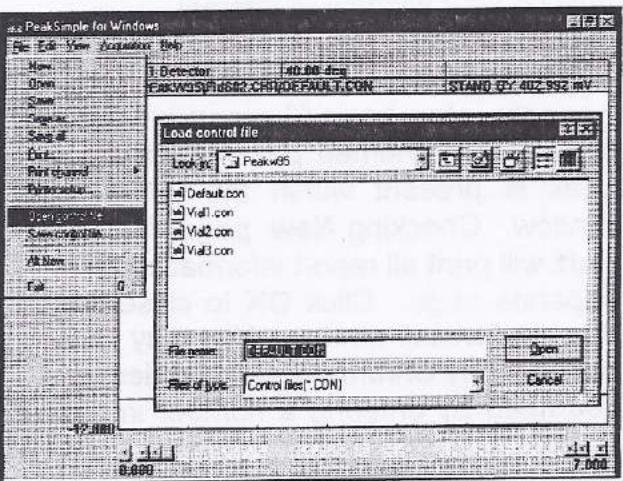
## The FILE-PRINTER SETUP Pull-Down Menu

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.

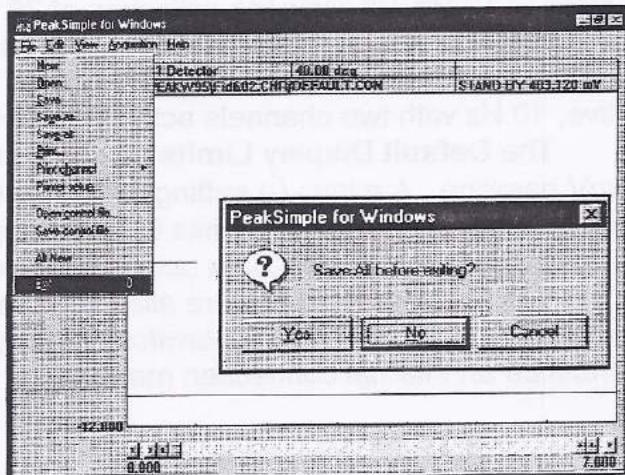
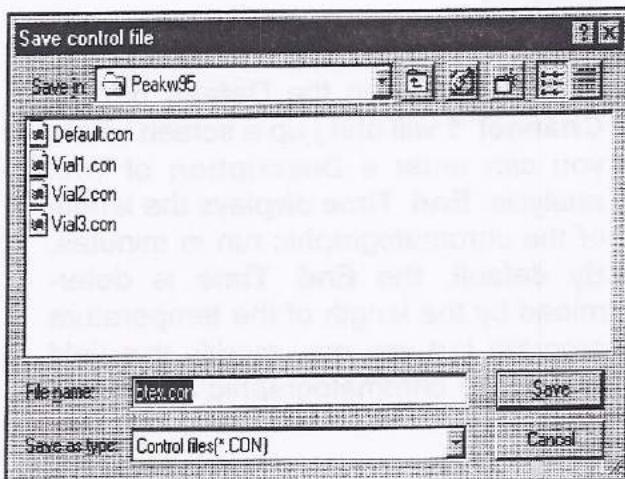
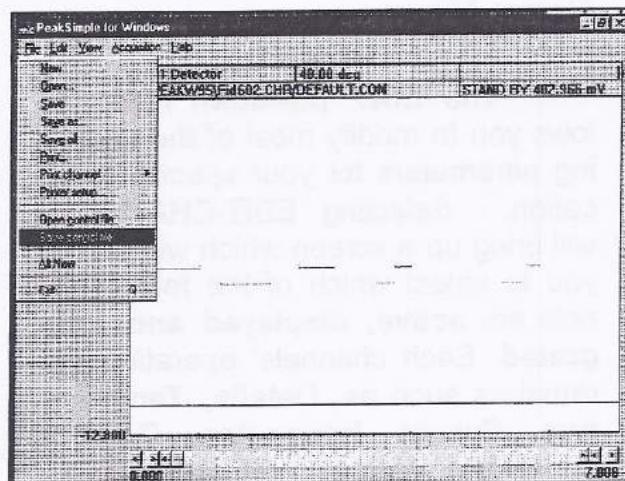
A **control file** is like a photocopy of your operating settings that you can reload for use at any time. When using **control files**, you only need to set analysis parameters once and then save them using a descriptive filename, followed by the **.CON** extension, (for example, **BTEX.CON** ). To 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 **Alternate** 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.

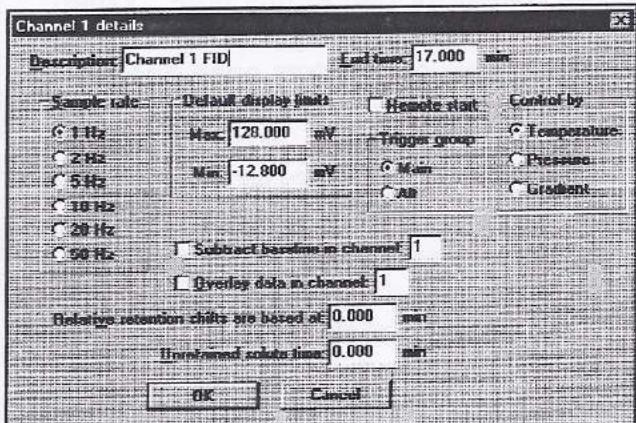
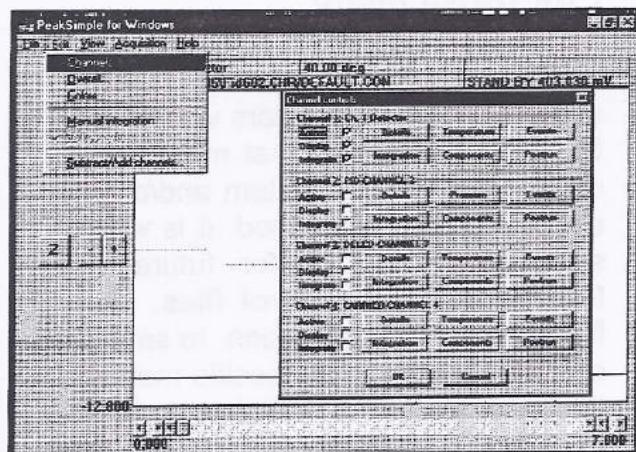


## The EDIT-CHANNELS Pull-Down Menu

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.

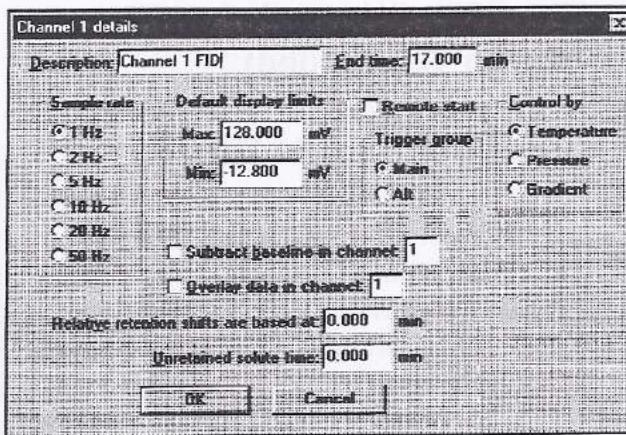
The **Default Display Limits** can be adjusted to view data above and below the 0 mV baseline. A minus (-) setting for **minimum** will display negative going peaks. The ratio of **min./max.** display limits is maintained when you click on the **Display** minus and plus buttons in the main data acquisition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

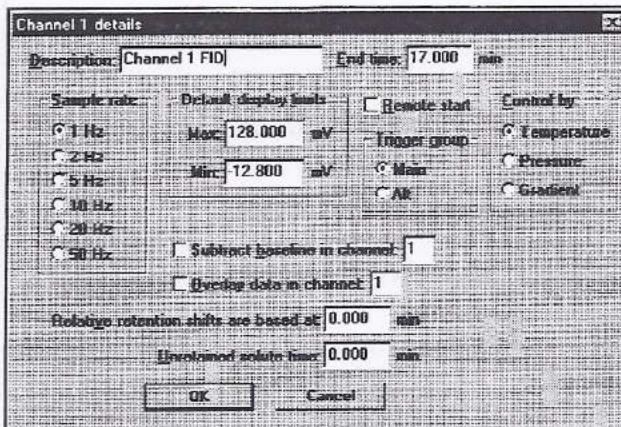
### Relative Retention Shifts Are Based At "X" Minutes

**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

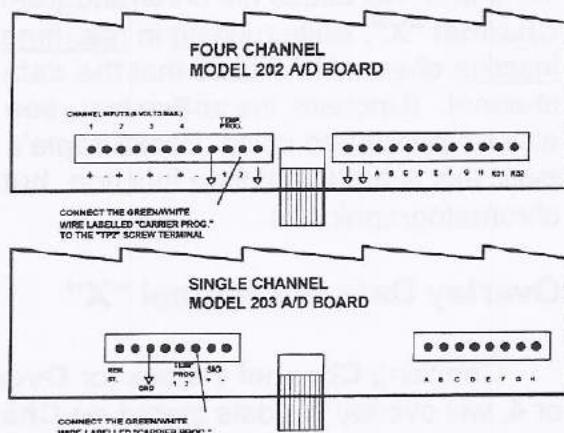
If resolution has been selected to be printed in the chromatogram report, then a **Unretained Solute Time** value needs to be entered to ensure correct resolution calculations. Enter the number of minutes an **Unretained Solute** takes to pass through the column. This value is used in the determination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

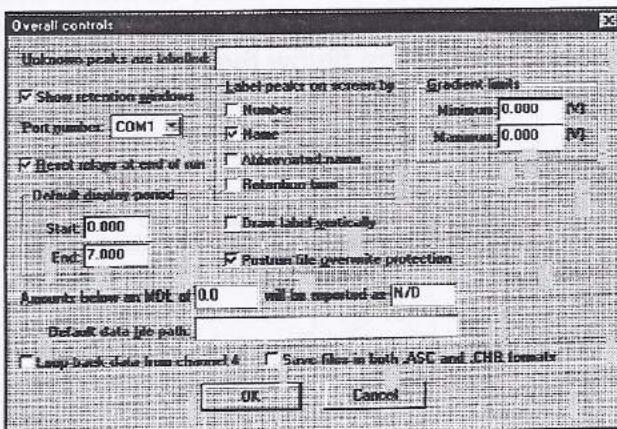
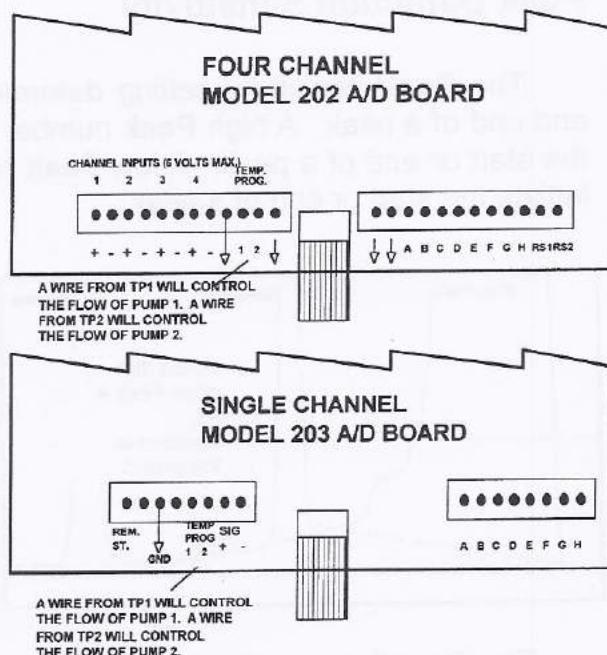
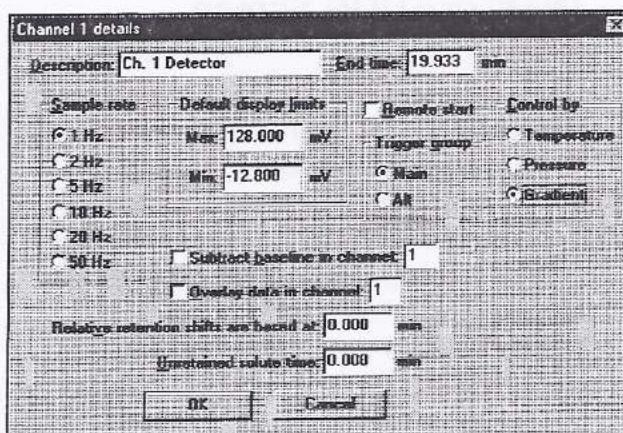
### Setting Up Gradients for Liquid Chromatography

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%.

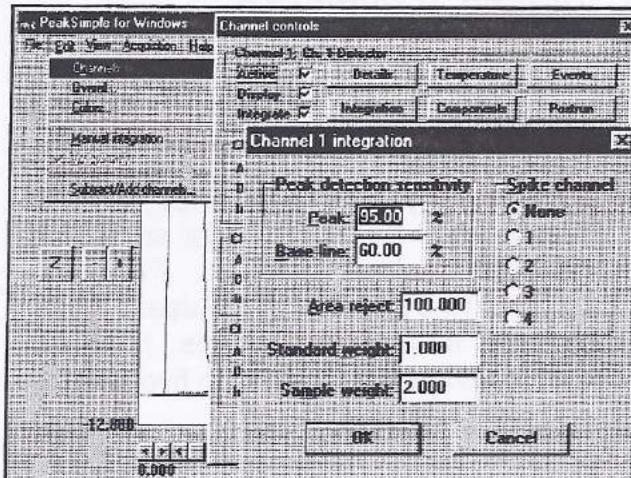
**Gradient Limits Zero** and **Span** may be scaled in the **Edit-Overall** screen to account for any offsets. PeakSimple allows for a voltage offset and scaling factor in these fields to calibrate the voltage output to match the pump's requirements.



## The EDIT-CHANNELS-INTEGRATION Screen

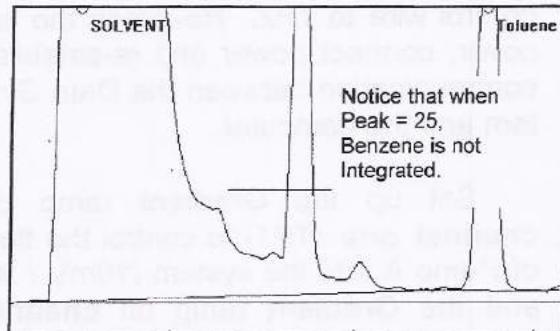
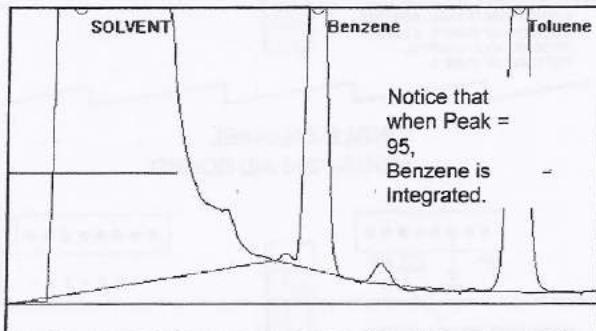
PeakSimple for Windows allows you to define specific integration parameters necessary for the proper analysis of your sample data, such as peak and baseline sensitivity and area reject. Any of the **Integration** parameters described below may be modified either before or after data collection.

Pressing the **ENTER** key will update the report and the results of the chromatogram currently being displayed.

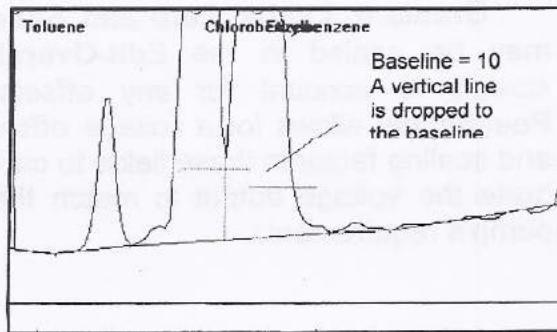
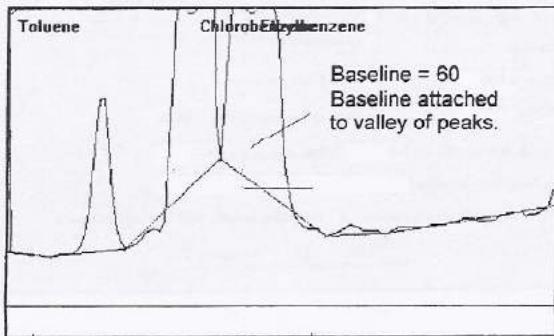


### Peak Detection Sensitivity

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.

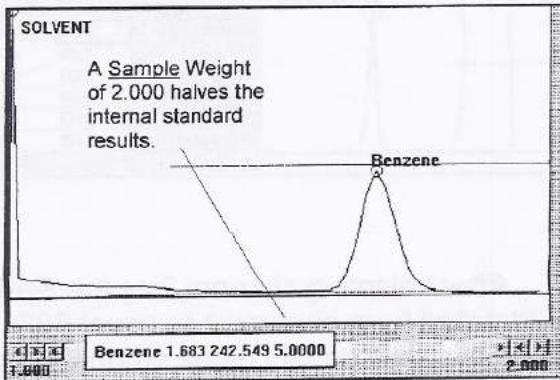
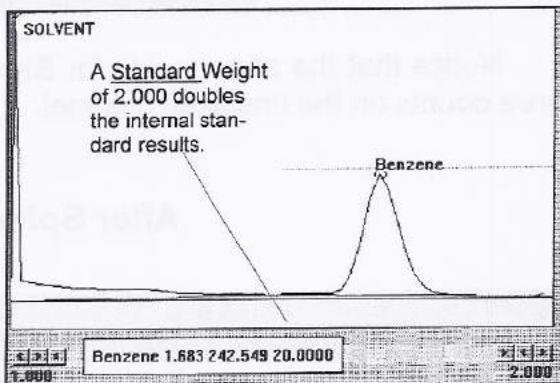
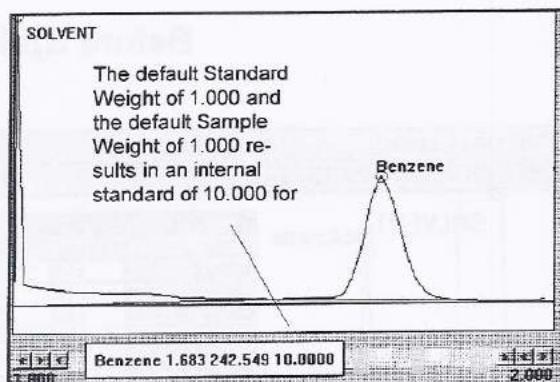
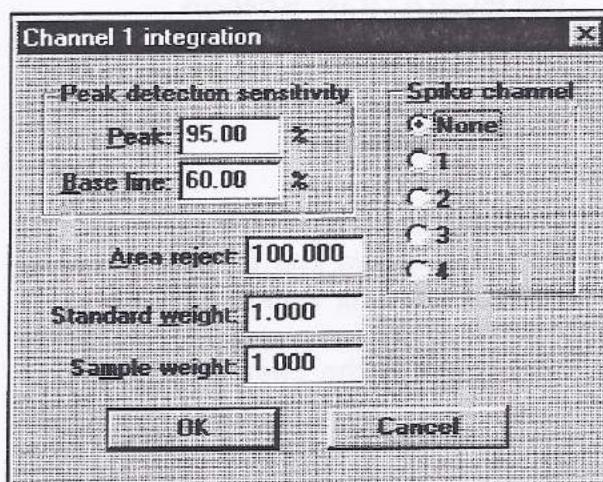
### Standard Weight

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

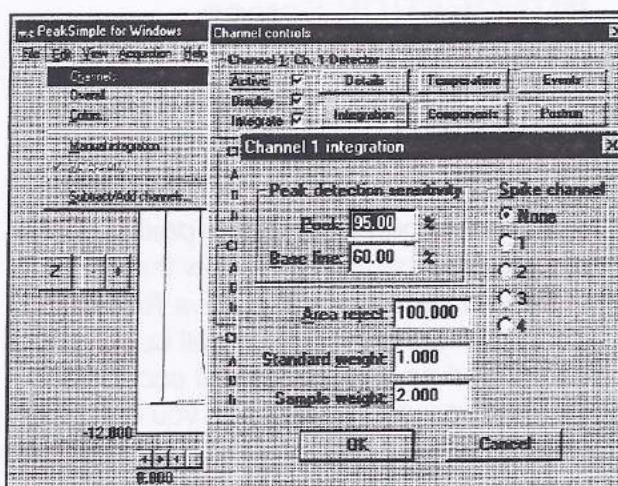
The **Sample Weight** setting may also be changed to adjust the channel's quantification, affecting internal or external peak results by the factor entered. For instance: A setting of 2.000 will double the weight of the sample thereby halving the internal or external standard results. (Decreased to 5.000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



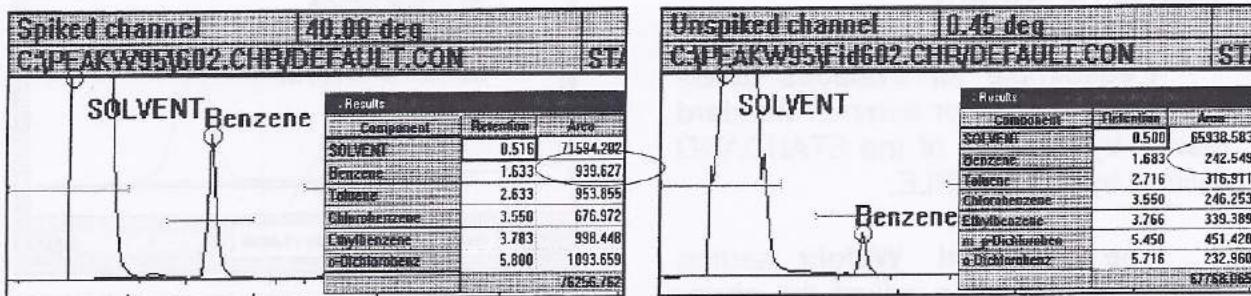
## The EDIT-CHANNELS-INTEGRATION Screen (continued)

### 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.

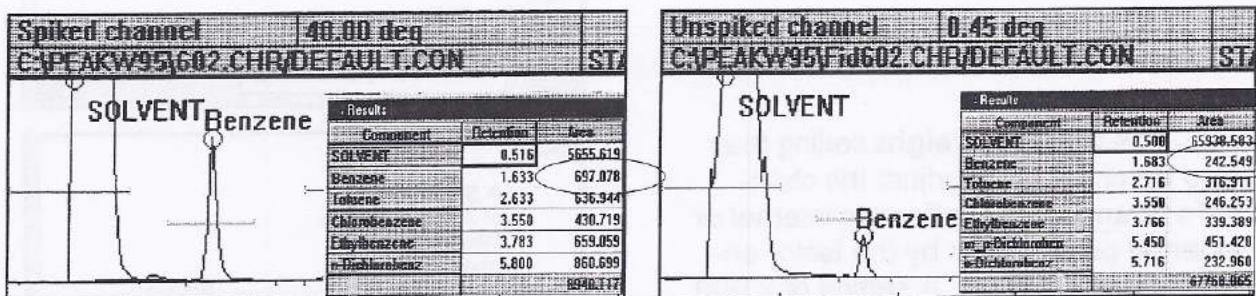


### Before Spike Channel Subtraction



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.

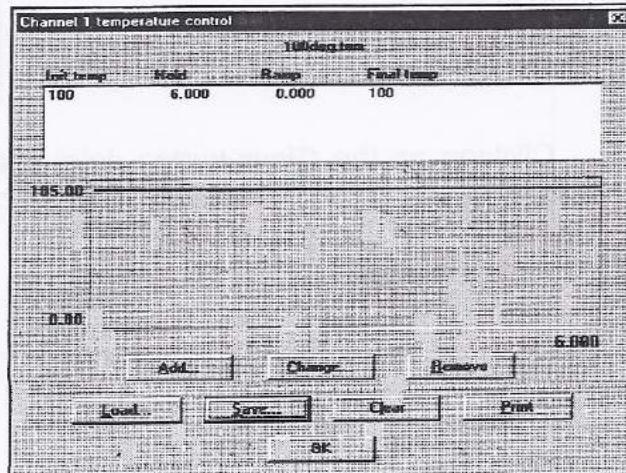
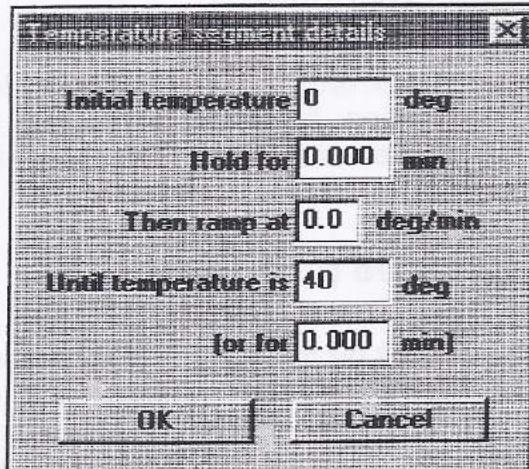
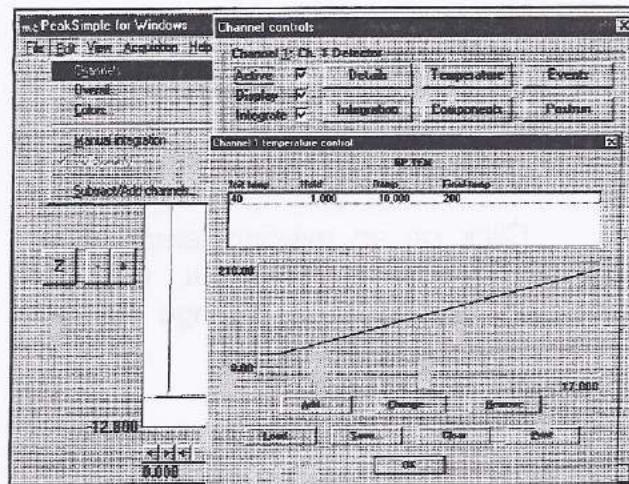
### The Temperature Segment Details Screen

#### 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

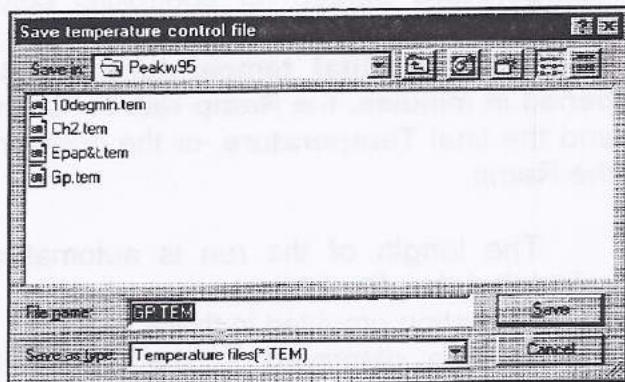
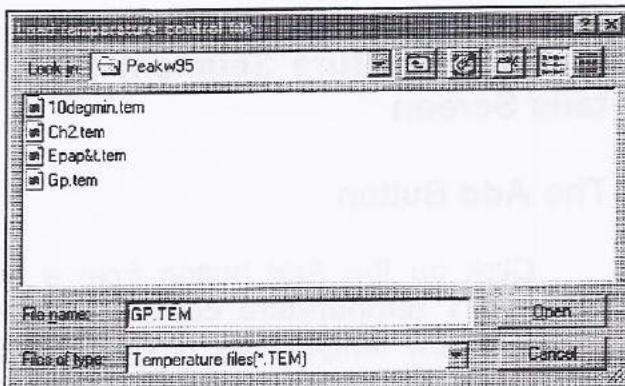
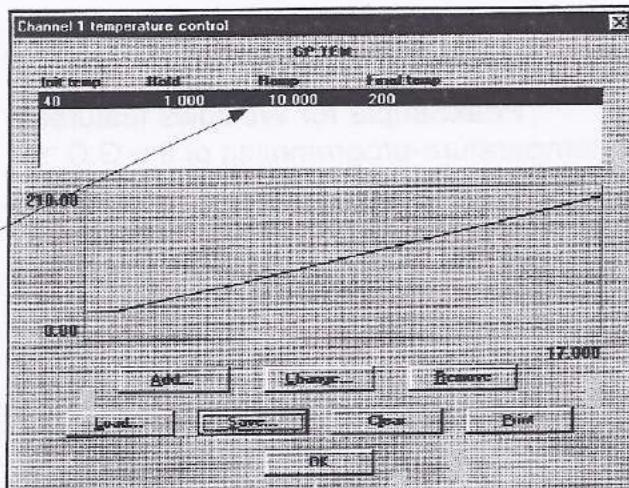
Click on the **Save** button to save a new temperature control file, or to update an existing one. Remember to use the **.TEM** extension when naming the temperature control file. The saved file name appears at the top of the temperature control window indicating the file in use.

### 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.



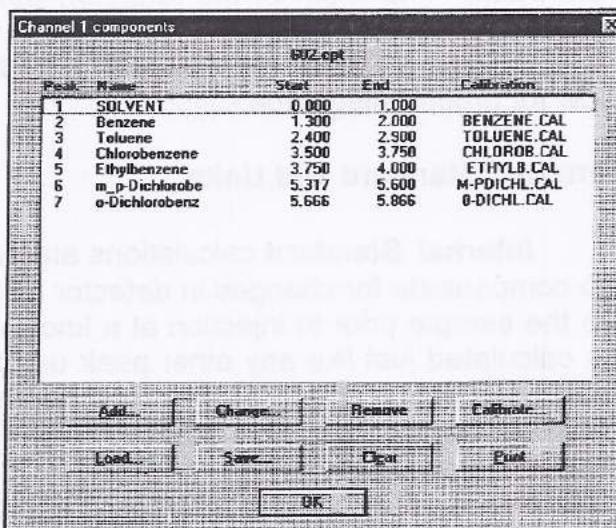
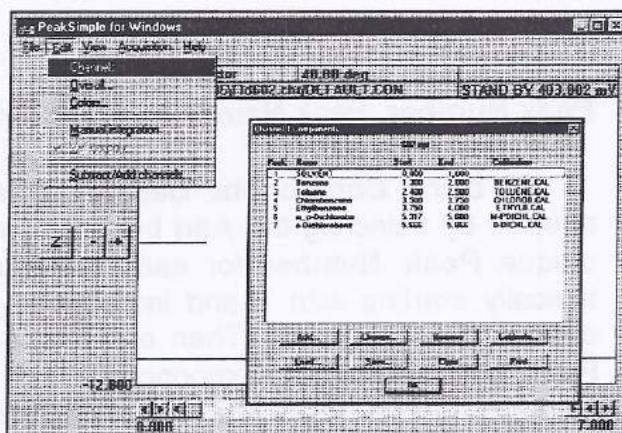
## The EDIT-CHANNELS-COMPONENTS Screen

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

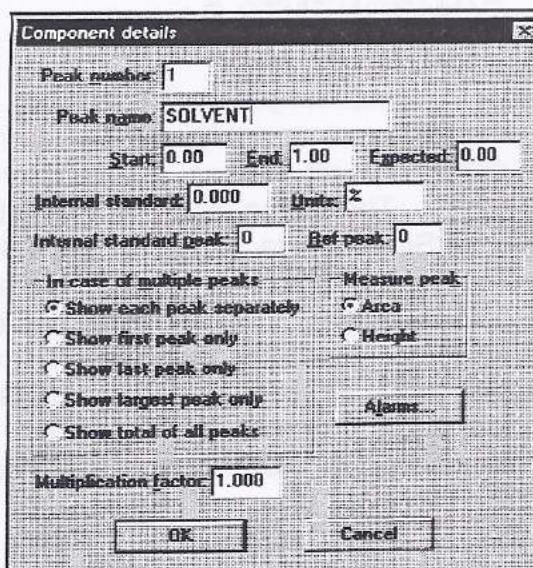
Select **Add** to add a new component to a blank or existing component table. The Component Details screen will open allowing the user to input specific peak parameters. As a minimum, enter the **Peak Number**, **Peak Name**, **Start** time and **End** time. Other optional parameters are the **Expected** 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  $104.95 \times 100/104.95$ . 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.

