



GC-LC Innovations

THE OP System for ALL SRI GCs

PeakSimple Data Systems

With 1, 4, or 6 Channels of Data Acquisition

4-Channel 202 NOW!
Discontinued ~2016

Standard in every SRI
GC and HPLC system

For any Windows™ computer

PS continuously
> upgraded
as SRI GCs evolve !



PeakSimple



USB or serial port

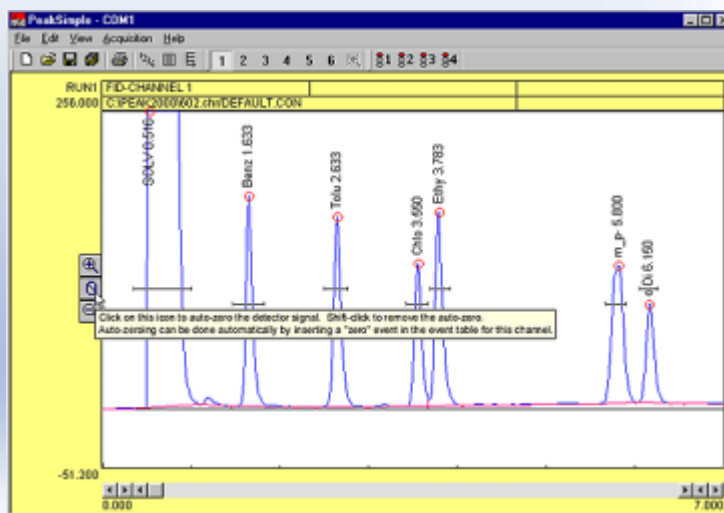


Available as a stand alone unit


SRI's PeakSimple Chromatography Data System is included with every SRI GC and HPLC system, and is also available as a convenient stand-alone data system for any other manufacturer's GC or HPLC. PeakSimple software has been continuously developed, refined and improved since 1988 by the same dedicated team of working chromatographers who use the software on a daily basis, and strive to simplify and enhance every aspect of PeakSimple so our customers will benefit. New features are added to PeakSimple several times per year and the latest version is always FREE to download online, along with helpful tutorials. Tech support at SRI is "old fashioned!" When you call, a knowledgeable technician will answer your questions right away. No complicated phone menus, and no waiting on hold!

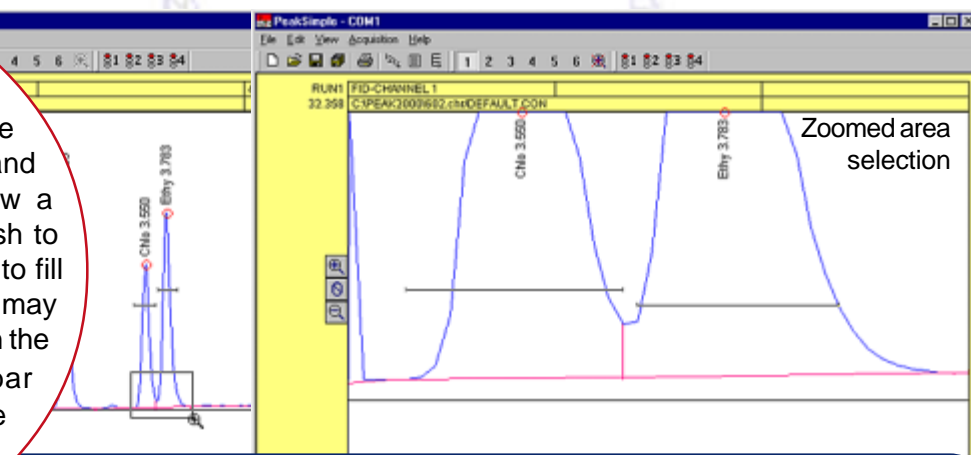
Easy to Learn, Easy to Use Software for all Windows™ Computers



Most PeakSimple functions are launched from the chromatogram window, and are so user friendly that most operators can produce results almost immediately. ToolTips makes learning your way around PeakSimple even easier—just hold your mouse cursor over any icon or checkbox to read the onscreen How-To instructions in one of many available languages.

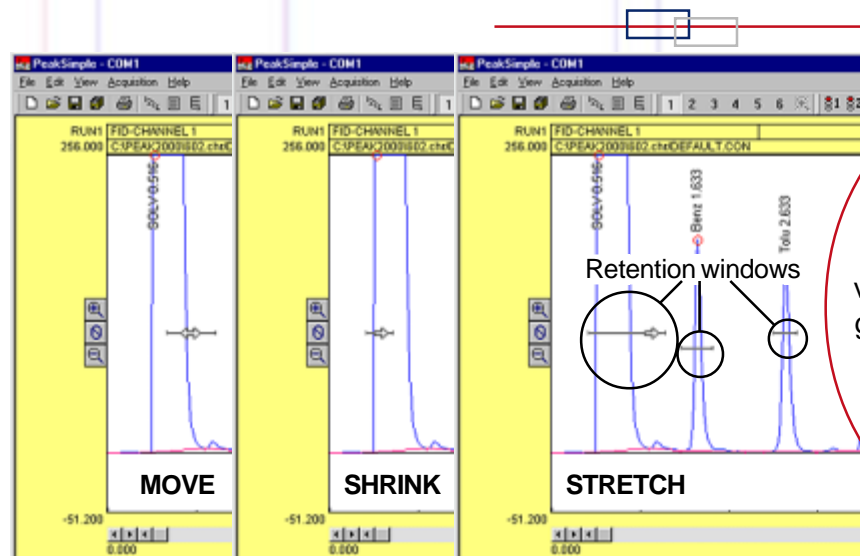


TAKE A CLOSER LOOK AT YOUR DATA

PeakSimple gives you two ways to closely examine data in the chromatogram window. Click and drag the mouse cursor to draw a rectangle around the area you wish to enlarge, and that area will expand to fill the chromatogram window. This may be done multiple times. Clicking on the Unzoom  icon in the toolbar unzooms one level at a time until you return to the original resolution.



A mouse click on one icon  vertically enlarges the peaks in the chromatogram, decreasing the y-axis display limits by a factor of two. A click on another icon  increases the y-axis display limits by a factor of two, which vertically shrinks the chromatogram peaks.



CLICK & DRAG RETENTION WINDOWS

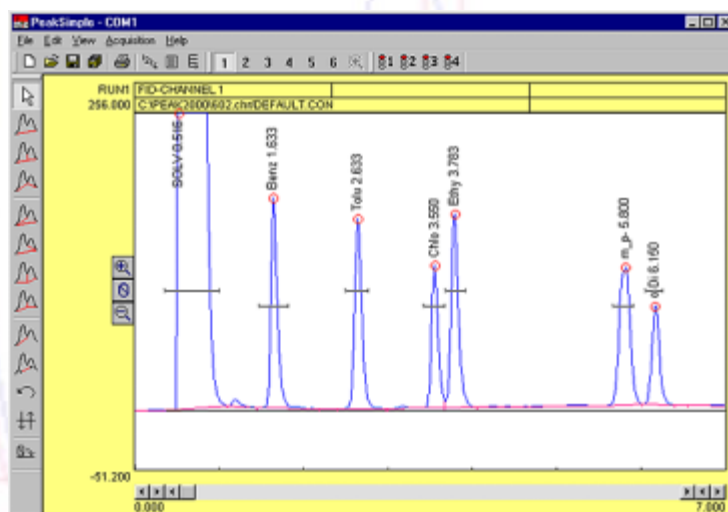
Retention window brackets are visible onscreen, and may be grabbed, dragged onto a peak, widened, or narrowed. The component table is automatically updated when a retention window is graphically moved or modified.

MANUAL INTEGRATION

Manual integration tools permit you to refine the integration method applied to any peak. The manual integration toolbox is available at a click of the mouse. Baseline projection may be “rubber-banded” from point to point, forced to a valley, dropped vertically, skimmed, etc.



The Manual Integration toolbox may be placed above (as shown at right) or to the left of the chromatogram window. It may also be dragged “off” the chromatogram window to float as an independent, move-able window.

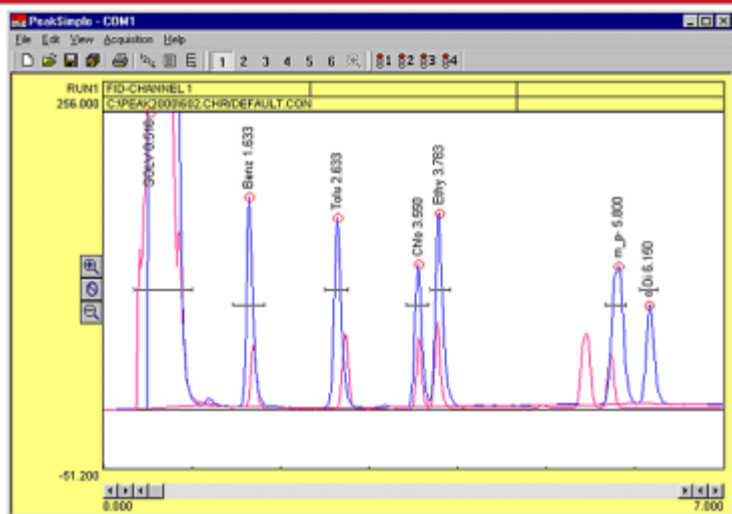


OVERLAY CHROMATOGRAMS

Overlay the data in any channel onto any other channel for retention time comparison or multi-detector correlation.

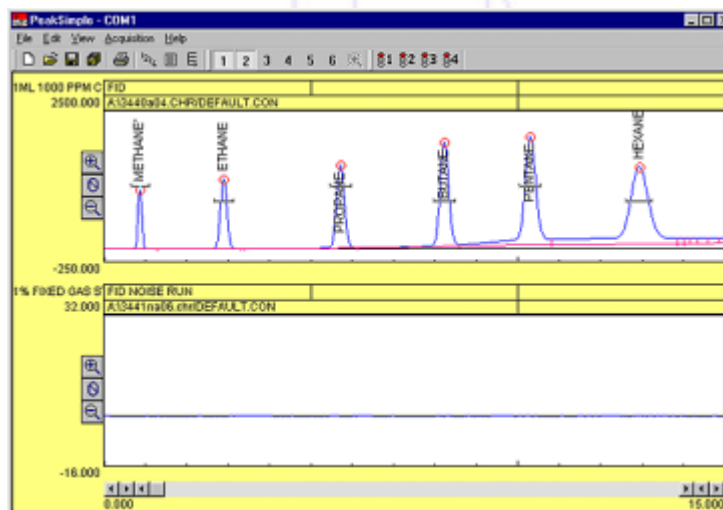


The Overlay Adjust feature lets you stretch and shift overlaid data to facilitate pattern matching.

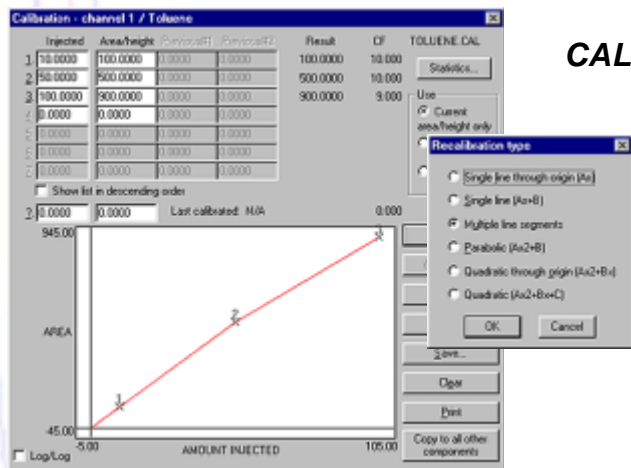
**BASELINE SUBTRACTION and DATA SMOOTHING**

Blank baseline subtraction is useful to compensate for baseline drifting due to column bleed and temperature ramping. PeakSimple lets you subtract baselines in real time as data is collected or post run.

Noisy detector signals can be smoothed manually or automatically at the end of a run. Smoothing algorithms include Olympian, Moving Average, and Savitsky-Golay.

**CALIBRATION****Multi-Level Calibration Curves**

Calibrate peaks six ways (multi-line, quadratic, parabolic, etc.) using single or averaged data at up to seven concentration levels. Statistics for evaluating line fit quality, modification date audit trail, and curve printout help to ensure defensible results.

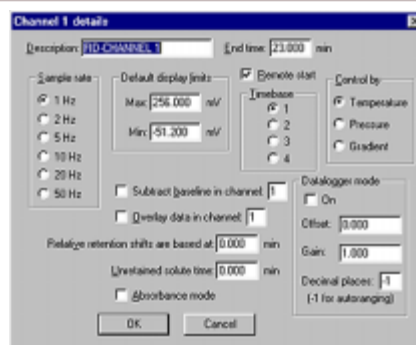
**Calibration Averaging**

PeakSimple allows up to three replicate calibration standards at seven levels of concentration to be averaged when constructing calibration curves.

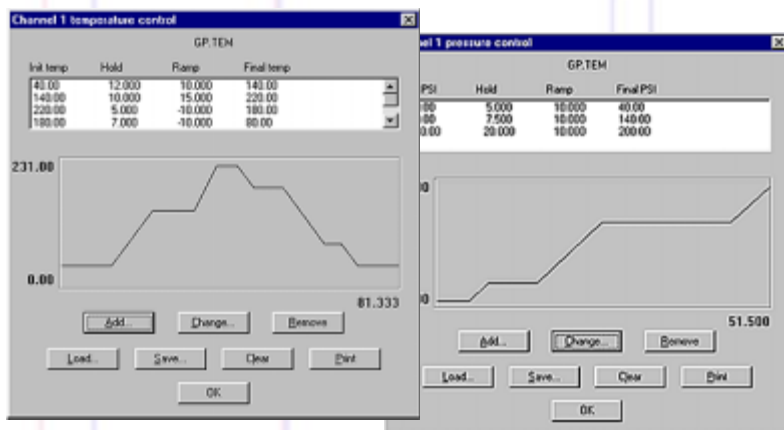


CHANNEL DETAILS

Each channel has a Channel details dialog box which allows users to set parameters for that particular channel. From the Channel details dialog box, you can set your sampling rate and default millivolt display limits; choose temperature, pressure, or gradient control; subtract the baseline from another channel; overlay the data from another channel; turn Data-logger mode ON or OFF; designate a start time to compensate for relative retention shifts, and more.



TEMPERATURE PROGRAMMING



EPC & HPLC GRADIENT PROGRAMMING

“Temperature,” “Pressure,” and “Gradient” channel control options all use the same simple dialog box, and each may be programmed with unlimited ramps and holds. Program one or two SRI GC column ovens from ambient to 400°C with 0.01 degree resolution and negative programming. Program the carrier gas pressure on SRI GCs equipped with electronic pressure control. Form binary HPLC gradients for low-cost pump control.

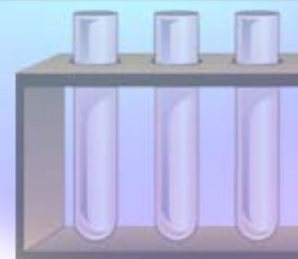
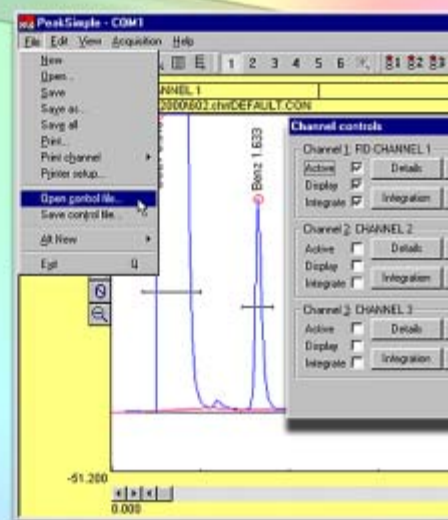
MANUAL/AUTOMATIC EXTERNAL EVENT CONTROL

In addition to performing timed integration events, control up to eight external contact closure relay outputs to actuate sampling valves, autosamplers, solenoids, pumps, or any external device using TTL or relay contact closure triggers.



CONTROL

Eliminate the need to repeat... simply by opening a control file. Maximize reproducibility—it does chromatograph because the control parameters. Save any change you make post-run actions, even color choices, to a control file for each method of analysis that control files you can have is limited only by you.





INTEGRATION

Use the Integration button to determine how PeakSimple integrates the data peaks in the chromatogram. Set peak detection sensitivity, area reject and standard weight. Specify a spike channel, merge results from another channel, and correct for sample weight and dilution.

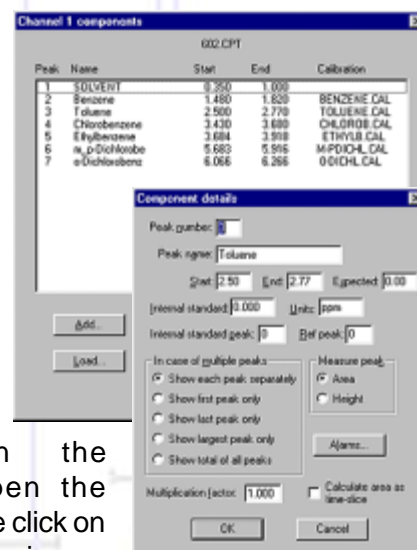
DL FILES

Specify run parameters before beginning an analysis. It doesn't matter who is operating the files contain all the necessary run parameters in the analysis, from channel details to control file and use it again and again. Create a file that your lab typically performs. The number of files on your disk space.



COMPONENTS

Create, save and edit component tables with an unlimited number of compounds. Enter expected retention times, control peak display, and more! Component details may be viewed and edited by double-clicking on any retention window in the chromatogram. Or, open the Component table and double click on any component in the list to view or edit that component's details.

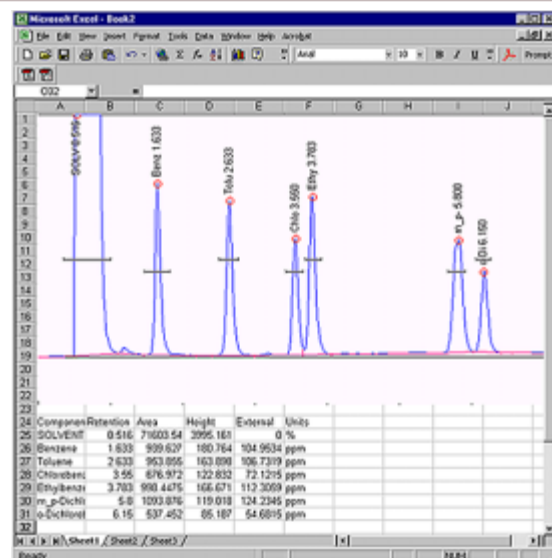


POSTRUN

PeakSimple can perform a variety of postrun actions to help you maintain and organize your data. Specify how data will be saved, and automatically add the results of the run to the results log for that channel. You can set PeakSimple to automatically print the results at the end of a run, and update your DDE link. Execute a command, specify a recalibration level, and restart the run after a given amount of time. You can even have PeakSimple smooth the data before copying it into another channel.

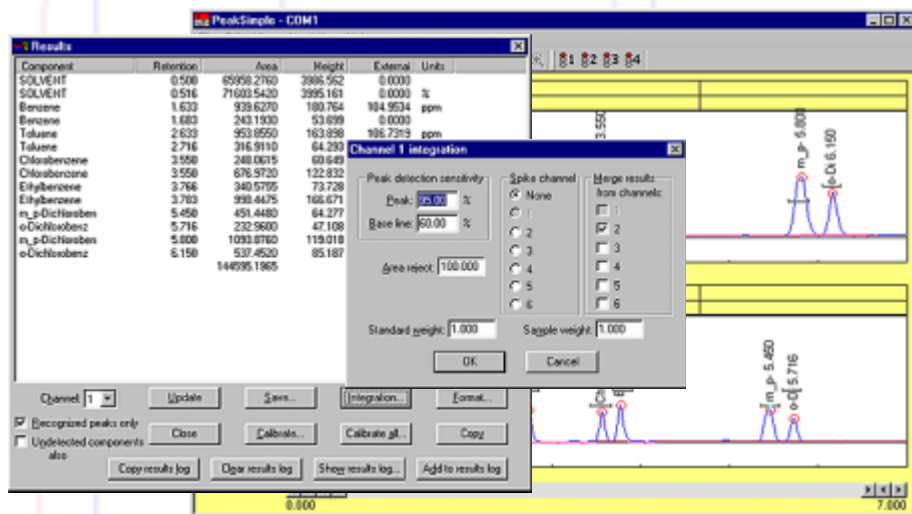
DYNAMIC DATA EXCHANGE

Link PeakSimple to your DDE compatible spreadsheet or word processor (Excel, Word, 123, etc.). Analytical results are automatically transferred after every run, or can be accumulated within PeakSimple and copied as a block of data. Use the Copy Picture option to paste the chromatogram itself into Excel, etc. along with the results.

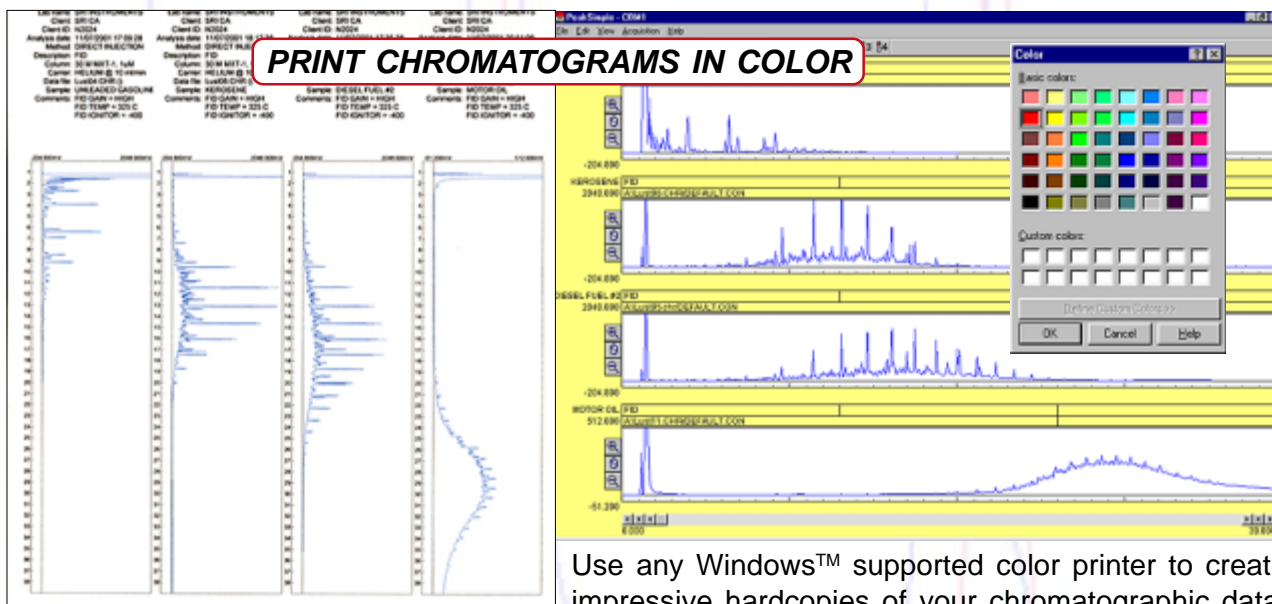


MERGE RESULTS FROM MULTIPLE CHANNELS

PeakSimple lets you merge the results from any channel or all channels into one report. This feature is handy when you're combining results from different detectors into a single report for export to Excel or other data analysis programs.



PRINT CHROMATOGRAMS IN COLOR



Use any Windows™ supported color printer to create impressive hardcopies of your chromatographic data. Print multiple chromatograms per page for easy detector-to-detector comparisons and paperwork consolidation. Print overlaid data in contrasting colors with adjustable line weight.

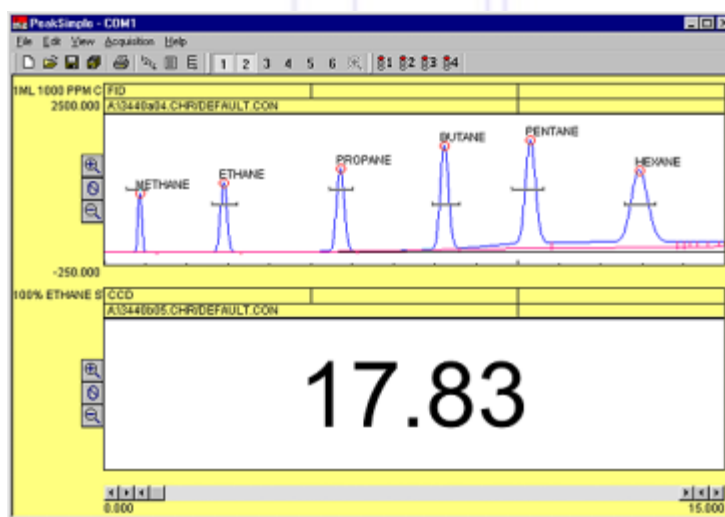


AUTOSAMPLER QUEUE and BATCH REPROCESSING

Create customized autosampler sequences for liquid injections, purge and trap autosamplers, gas sampling valves, and stream selectors including unique predefined sample information, auto-calibration and batch reprocessing of previously run samples.

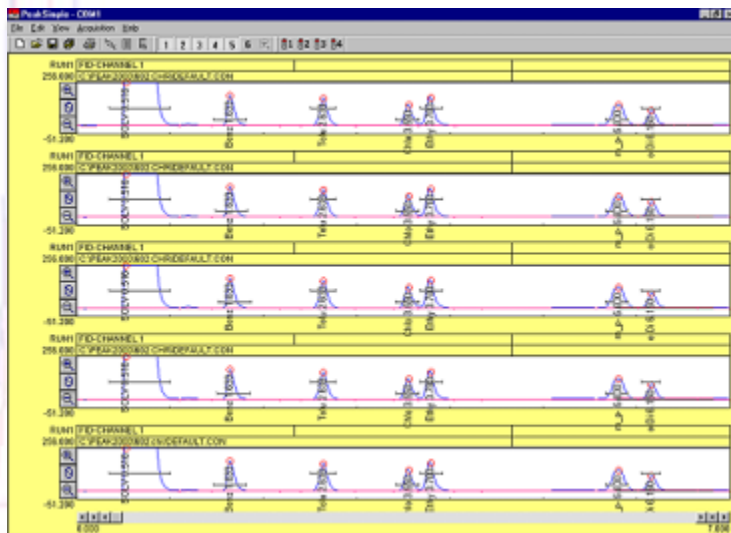
DATA LOGGER MODE

Peak Simple's Data Logger Mode allows you to display a scaled and calibrated result in large numbers instead of the usual strip chart data presentation. Data Logger Mode is especially useful when monitoring total hydrocarbons on one channel while performing a separation on another channel.



SELF-VALIDATING HARDWARE

PeakSimple will play back and re-acquire any chromatogram multiple times, establishing the precision and accuracy of the data system using real data, not "canned" chromatograms. PeakSimple's validation can be performed by the user anytime without extra hardware.



SRI PeakSimple Data Systems

Serial Port

Models 202 and 203 connect to your computer with a serial port cable. Windows™ computers with two available serial ports can operate dual **203** systems, a **202** and **203** together, or dual **202** systems for a total of up to eight data channels and four time bases. Temperature and pressure control outputs are available for connection to a GC or HPLC. PeakSimple software works with each of the following hardware options, serial or USB port, and is included with each unit.

Model 203 has one channel capable of acquiring data at up to 50Hz. Its eight TTL outputs can be optionally wired to a bank of eight single-pole, dual-throw mechanical relays with screw terminals for easy connection to any user device which operates from a contact closure. A remote start input allows run initiation from the user's GC or HPLC system. The 220VAC system is supplied with a UL, CSA, and CE/VDE approved universal voltage input which will operate on any 100-250 volt power supply.

Model 203



Approximately 8" wide x
8" deep x 1.75" high

Model 202 has four channels. Data can be acquired at up to 50Hz with one channel active, 10Hz with two channels, or 5Hz with all four channels activated. assigned to one of two times for two entirely allow run initiation from the user's GC or HPLC system. Model 202 includes the bank of eight single-pole, dual-throw mechanical relays with screw terminals for easy connection to any device that operates from a contact closure.

Model 202

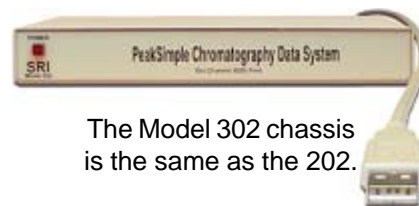


Approximately 15" wide x
11" deep x 2" high

USB

Model 302 is for analysts who prefer the hot-swappable, plug-and-play capabilities of Universal Serial Bus devices. Four remote start inputs allow run initiation from the user's GC or HPLC system. The six channels of data can be randomly assigned to one of four time bases which provides independent start and stop times for 4 entirely separate instruments. Data can be acquired at up to 50Hz per channel with 4 channels active, and up to 20Hz with all 6 channels activated and acquiring data. The Plug and Play peripheral connection of choice, USB is supported by Microsoft Windows 98, 98SE, ME, XP, and 2000.

Model 302



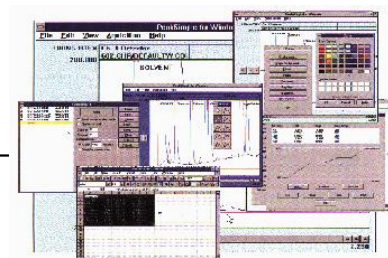
The Model 302 chassis
is the same as the 202.

8600-1055	Model 203 Single Channel Data System with PeakSimple software	\$ 1,395.00
8600-1255	Model 203 220VAC	\$ 1,495.00
8600-4055	Model 202 Four Channel Data System with PeakSimple software	\$ 2,395.00
8600-4255	Model 202 220VAC	\$ 2,395.00
8600-6055	Model 302 Six Channel USB Data System with PeakSimple software	\$ 2,595.00
8600-6255	Model 302 220VAC	\$ 2,595.00

Model 302 Six Channel Data System



For SRI GC Control OR as Stand-alone independent 6-Channel Data System



- **6 channels, 4 separate time bases, 4 remote start inputs**
- **Independent start & stop times for 4 separate instruments**
- **USB 2.0 connection to your Windows™ PC**
- **Includes PeakSimple software**

The Model 302 is available mounted inside the 8610C, 8610D, 410, and 310 GCs, or it can be mounted in a separate box for connection to other manufacturers' GC or HPLC detectors.

The Model 302 data system consists of PeakSimple chromatography software for Windows, and a six channel, 20-bit high resolution A/D board.

When mounted in a SRI GC, the Model 302 controls the column oven temperature program, and the pressure program of the carrier gas electronic pressure controller (EPC).

The eight available TTL outputs are connected internally within the GC to control functions like valve rotation, gas solenoid actuation, autosampler injection, etc.

When mounted in a separate box, the temperature, pressure, and gradient control outputs are available for use, but not connected to anything.

The eight TTL outputs are wired to a bank of eight single-pole, dual-throw mechanical relays with screw terminals for easy connection to any user device which operates from a contact closure.

Four remote start inputs allow run initiation from the user's GC or HPLC system.


Each of the six channels of data can be randomly assigned to one of four time bases, which allows independent start and stop times for four separate instruments.

Data can be acquired at rates up to 50Hz per channel for one or two channels, or 20Hz for all six channels.

The Model 302 is for use with Windows computers that have USB 2.0 compliant ports.

8600-6055 Model 302 six channel USB data system USD3,180.00

8600-6255 Model 302, 230VAC USD3,180.00




GC-LC Innovations

PeakSimple Data Systems


With 1, or 6 Channels of Data Acquisition

Standard in every SRI GC and HPLC system




USB or serial port

For any Windows™ computer



Available as a stand alone unit



Model 302 Six Channel USB Chromatography Data System Quick Start Tutorial

The Model 302 comes with a two meter USB cable, power cord, (may be either 120 or 220 volt) and a PeakSimple software disk. PeakSimple software may also be downloaded from www.srigc.com. Its a good idea to check the website in case a more recent software version has been released.

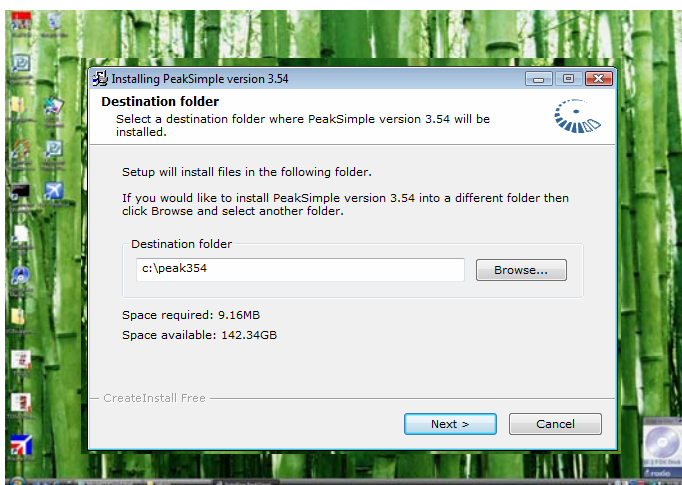
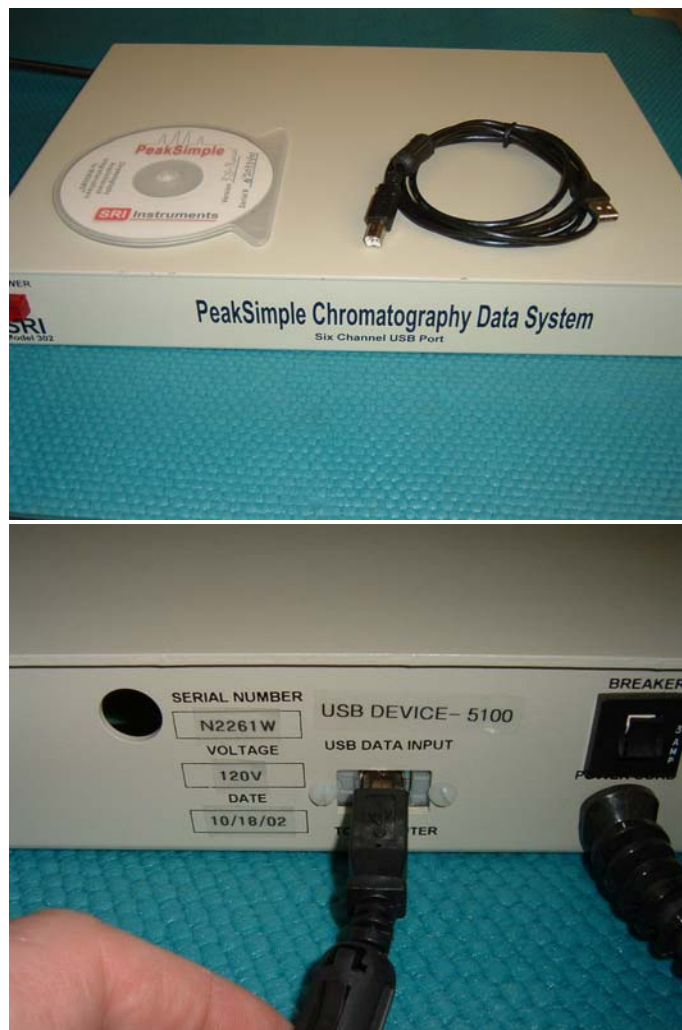
If the 302 A/D board is installed in a SRI GC rather than in a stand-alone box as shown then plug the USB cable into the right side of the GC. Also, if the 302 is installed in an SRI GC then all of the hardware connections will have been made already, you just have to install the software.

Plug the power cord from the 302 box into the mains wall socket and turn on the power switch located on the back of the stand-alone box. Plug the USB cable into the 302 box.

Wait until PeakSimple software is already installed before plugging the USB cable into your computer.

Install PeakSimple software from the CD disk or from the file downloaded from SRI's website. Browse to the CD or to the downloaded file on your hard-drive (C:\) . The file's name will be setup354 if it is version 3.54 of PeakSimple and setup356 if the PeakSimple version number is 3.56. PeakSimple is updated every few months usually to add a new feature.

Install PeakSimple in the suggested folder (C:\peak354) unless you have a very good reason to choose another. Using the typical folder name helps simplify the tech support process.



Model 302 Six Channel USB Chromatography Data System Quick Start Tutorial

When you click "Next" the PeakSimple software will be installed and you will see the screen to the right. Click "Finish"

Now connect the USB cable to your computer.

A hardware "Wizard" will appear to help you install the USB driver. The example shown is for a Vista operating system. **For XP computers the "wizard" screens will be slightly different.**

Follow the screens as shown

At the end of the process you can verify that the driver was installed by looking at the "Device Manager" screen in the "Control Panel"

PeakSimple version 3.54 has been successfully installed!

Click Finish to complete the installation.

Found New Hardware

Windows needs to install driver software for your sri333

Locate and install driver software (recommended)
Windows will guide you through the process of installing driver software for your device.

Ask me again later
Windows will ask again the next time you plug in your device or log on.

Don't show this message again
Your device will not function properly.

Found New Hardware - sri333

Insert the disc that came with your sri333

If you have the disc that came with your device, insert it now. Windows will automatically search the disc for driver software.

Found New Hardware - sri333

Windows couldn't find driver software for your device

Check for a solution
Windows will check to see if there are steps you can take to get your device working.

Browse my computer for driver software (advanced)
Locate and install driver software manually.

Browse for driver software on your computer

Search for driver software in this location:
C:\peak354

Include subfolders

Found New Hardware - sri333

The software for this device has been successfully installed

Windows has finished installing the driver software for this device:

Found New Hardware - sri333

Windows Security

Windows can't verify the publisher of this driver software

Don't install this driver software
You should check your manufacturer's website for updated driver software for your device.

Install this driver software anyway
Only install driver software obtained from your manufacturer's website or disc. Unsigned software from other sources may harm your computer or steal information.

See details

Select Install Anyway

Found New Hardware - sri333

The software for this device has been successfully installed

Windows has finished installing the driver software for this device:

Found New Hardware - sri333

Windows Security

Windows can't verify the publisher of this driver software

Don't install this driver software
You should check your manufacturer's website for updated driver software for your device.

Install this driver software anyway
Only install driver software obtained from your manufacturer's website or disc. Unsigned software from other sources may harm your computer or steal information.

See details

Select Install Anyway

Device Manager

View Insert Format Tools Table Arrange Window Help Adobe PDF

File Action View Help

Mice and other pointing devices

Modems

Monitors

Network adapters

Ports (COM & LPT)

Processors

Sound, video and game controllers

Storage volumes

System devices

Universal Serial Bus controllers

Intel(r) 82801DB/DBM USB 2.0 Enhanced Host Controller - 24C2

Intel(R) 82801DB/DBM USB Universal Host Controller - 24C2

Intel(R) 82801DB/DBM USB Universal Host Controller - 24C4

Intel(R) 82801DB/DBM USB Universal Host Controller - 24C7

Lawson Labs, Inc. USB Data Acquisition Hardware

USB Mass Storage Device

USB Mass Storage Device

USB Root Hub

USB Root Hub

USB Root Hub

USB Root Hub

USB Root Hub

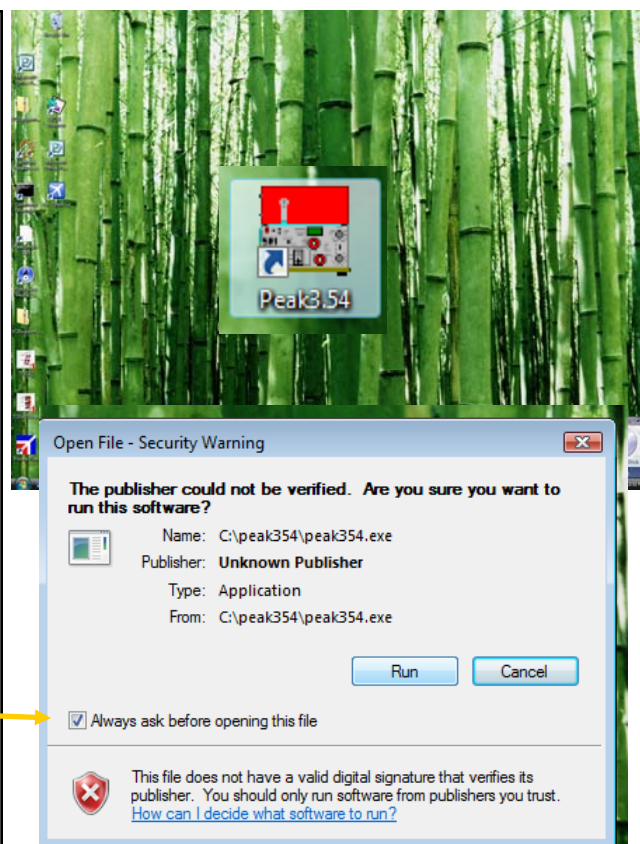
Under the Universal Serial Bus Controllers See Lawson Labs listed

Model 302 Six Channel USB Chromatography Data System Quick Start Tutorial

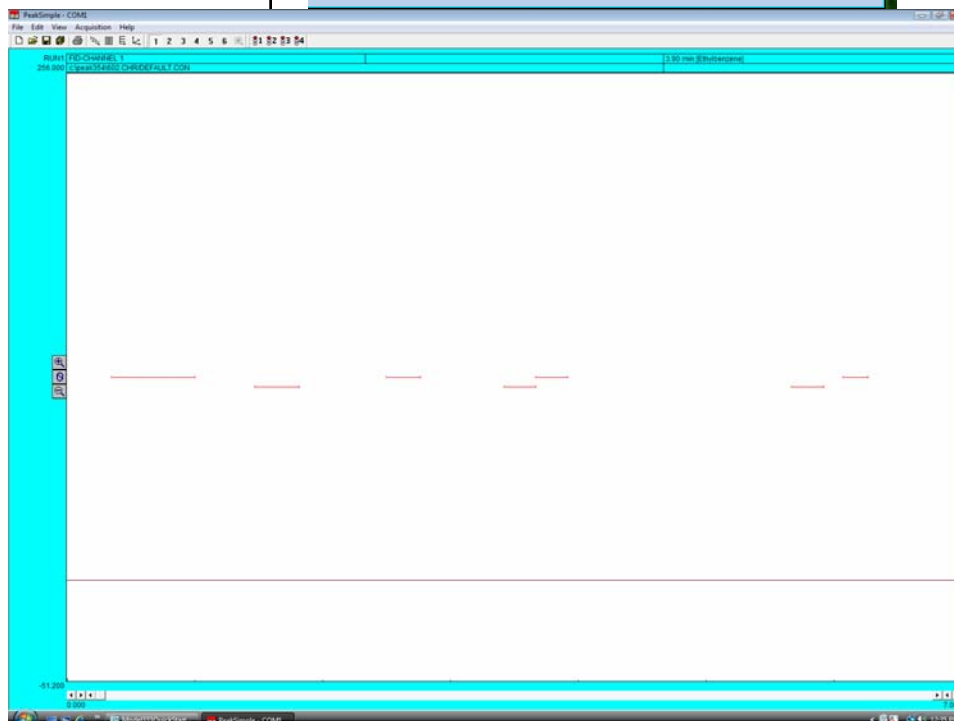
Click on the PeakSimple icon (which will be somewhere on the Windows Desktop screen) to launch PeakSimple.

This warning will appear, but click "Run " anyway.

You can un-check this box to avoid this message in the future.



The PeakSimple screen will look like this.



Model 302 Six Channel USB Chromatography Data System Quick Start Tutorial

Use your mouse to click on "Edit" and then "Overall..."

In the "Overall..." screen enter the "Board Type" (302) and then the "USB device number".

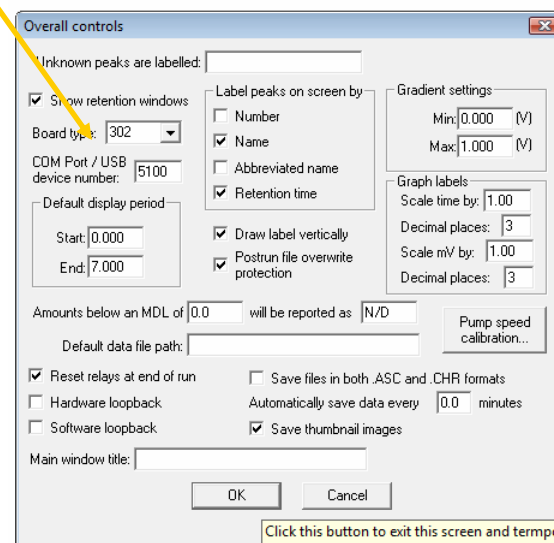
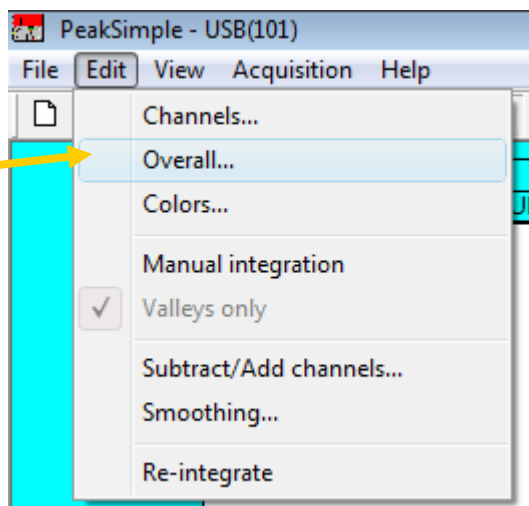
The USB device number is a unique number which identifies this particular 302 board. Because each 302 board has a unique number you can operate several of them independently on one single computer . The USB device number is printed on the back of the 302 box and also on the USB controller chip on the 302 board.



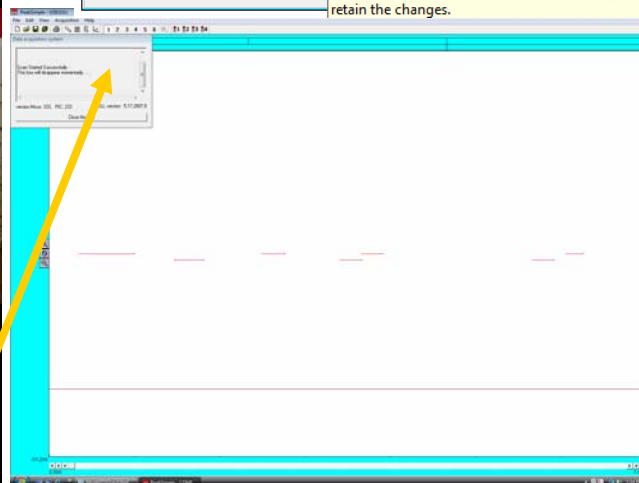
On a GC the device I.D.# is printed next to the USB jack on the side on the instrument.



When you click "OK" you will see a box on the top left of the screen which displays the calibration conversation PeakSimple has with the Model 302 board.



Click this button to exit this screen and temporarily retain the changes.



Model 302 Six Channel USB Chromatography Data System Quick Start Tutorial

Use your mouse to click on "Edit" and then "Channels" or just click on the "Channels Icon" which looks like the numbers 1,2,3,4.

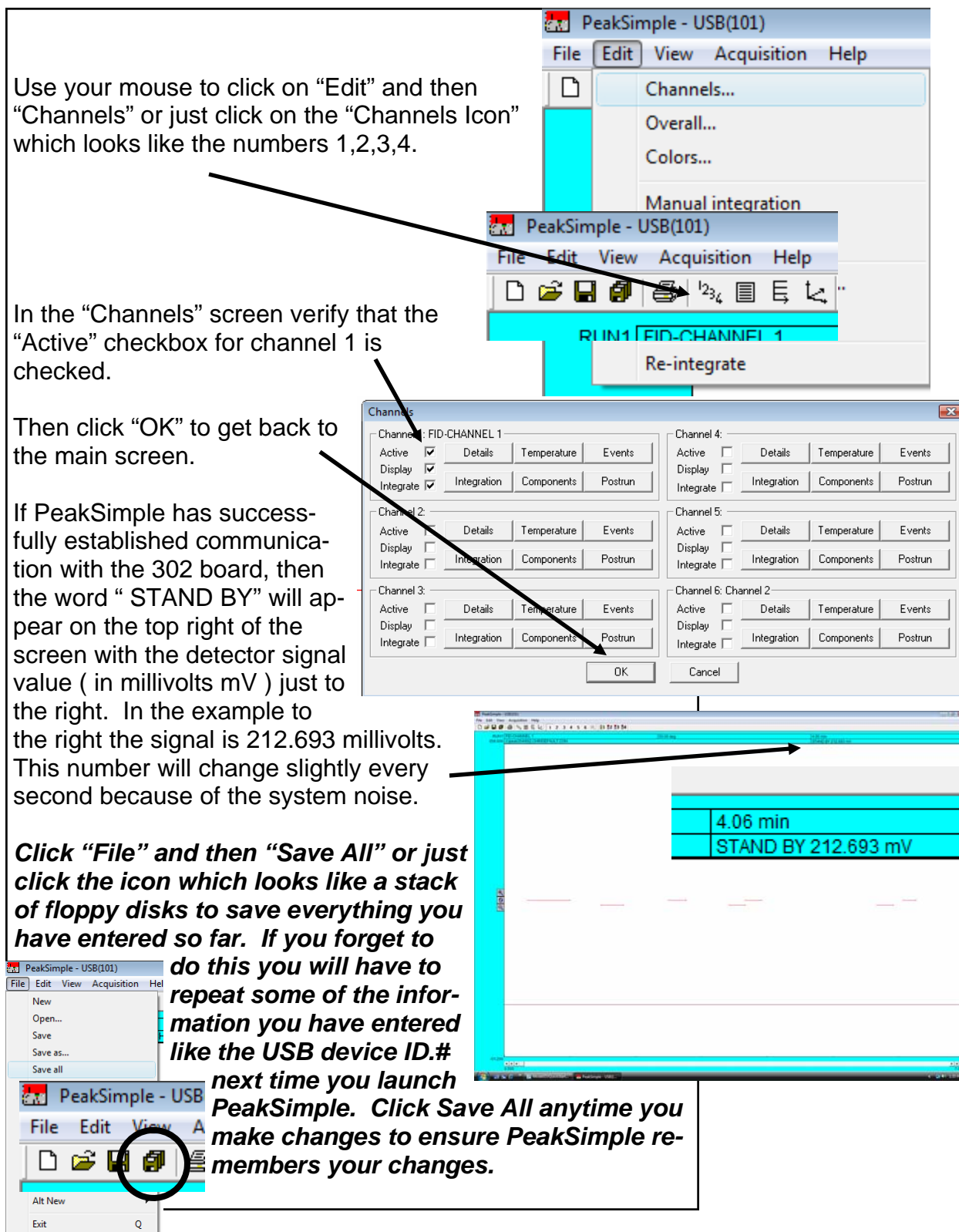
In the "Channels" screen verify that the "Active" checkbox for channel 1 is checked.

Then click "OK" to get back to the main screen.

If PeakSimple has successfully established communication with the 302 board, then the word "STAND BY" will appear on the top right of the screen with the detector signal value (in millivolts mV) just to the right. In the example to the right the signal is 212.693 millivolts. This number will change slightly every second because of the system noise.

Click "File" and then "Save All" or just click the icon which looks like a stack of floppy disks to save everything you have entered so far. If you forget to do this you will have to repeat some of the information you have entered like the USB device ID.#

next time you launch PeakSimple. Click Save All anytime you make changes to ensure PeakSimple remembers your changes.



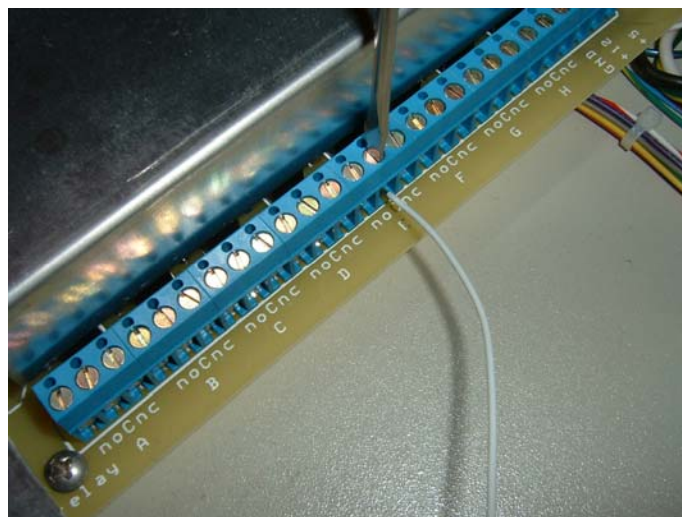
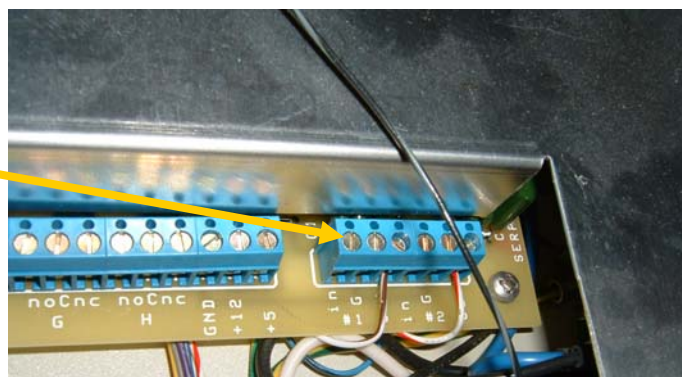
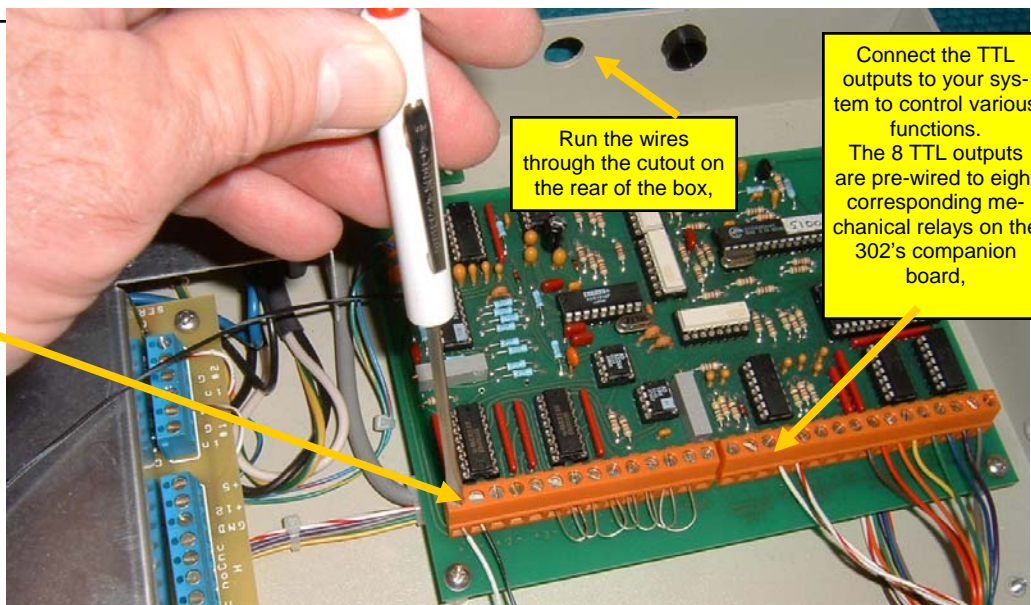
Model 302 Six Channel USB Chromatography Data System Quick Start Tutorial

Connect the detector signals to the 302 board using the terminals labeled In+ and In-. There are 6 sets of in+ and in- screw terminals

Choose the "Integrator", "Computer" or "Chart Recorder" output from your system. On attenuation 1, the "Chart Recorder" output is the same as the "Integrator" or "Computer" output.

Connect the "Remote Start" output from your instrument to the "in#1" (remote start) and G (ground) terminals on the 302 companion board. ***This step is OPTIONAL, you do not have to use the Remote Start feature..***

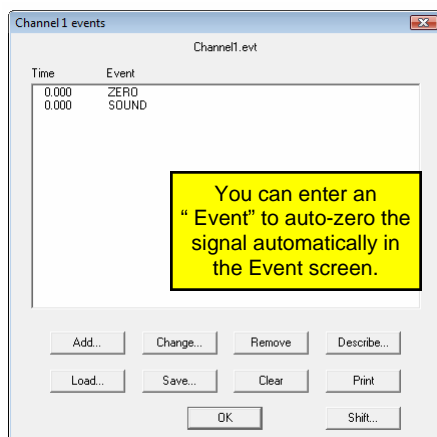
Connect the TTL (relay) outputs to your system. For example, if you wanted to actuate a Valco valve on your GC you could use the TTL outputs to trigger the valve. You may use either the TTL (0-5 volts DC) outputs located on the A/D board or any of the eight pre-wired mechanical relays located on the companion board. Each mechanical relay has a common (C), normally open (NO) and normally closed (NC) screw terminal. ***This step is also OPTIONAL, you do not have to use the TTL (relay) outputs..***



Model 302 Six Channel USB Chromatography Data System Quick Start Tutorial

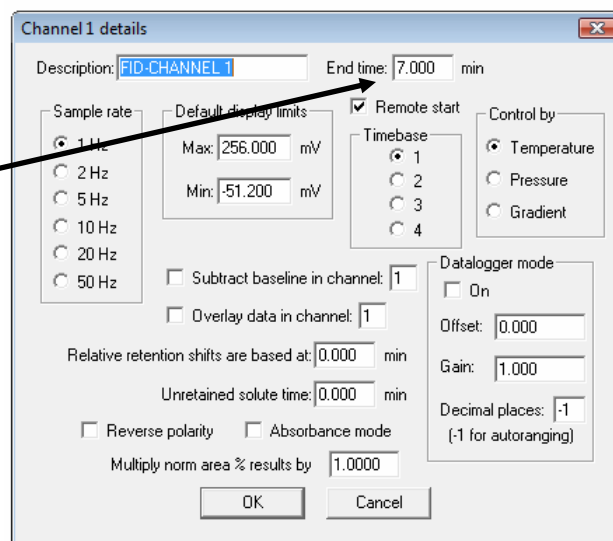
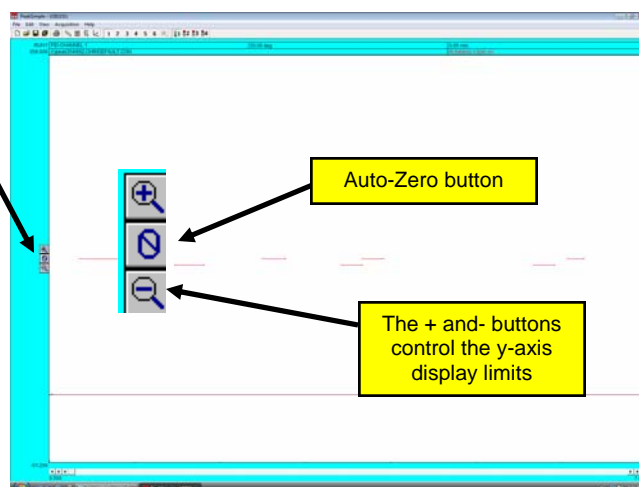
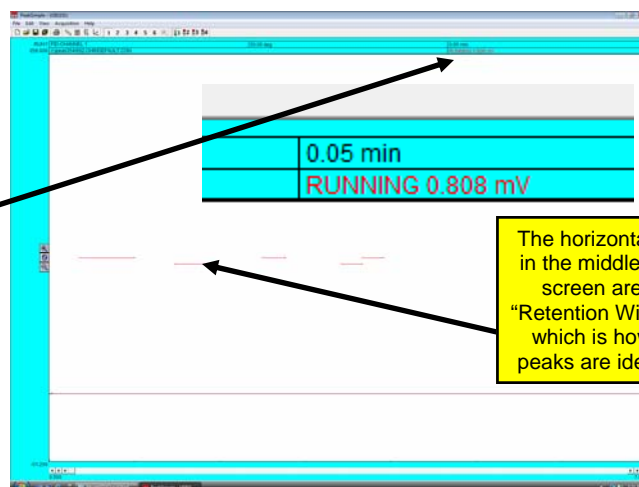
Press the "Spacebar" on your computer's keyboard to start the Run. (there are several ways to start the run including a "Remote Start"). The word " Stand By " will change to "Running" and the data line will be drawn on the strip-chart area of the main screen.

Click the Auto-Zero button to bring the signal down to 0.00 millivolts (there are several ways to auto-zero the signal including an "Event" in the Event Table which auto-zeros the signal automatically at the beginning of the Run).



The " Run " will end at the time specified in the Channel Details screen unless you end it earlier by depressing the " End " key on the keyboard.

For more information download the PeakSimple tutorials on www.srigc.com or call SRI Tech Support at 310-214-5092



Model 302

Six Channel USB PeakSimple Data System

The **Model 302** may be used with any brand or model of GC or HPLC offering an analog detector output signal ranging from -5V to +5V. It includes three independent, programmable controls (0V to +5V analog output) for temperature & pressure or HPLC gradient formation. The Model 302 has six channels, which can be randomly assigned to one of four time bases, which allows independent start and stop times for four separate instruments. Four remote start inputs compatible with 2-wire switch closures (typically output by GCs and HPLCs as a remote start signal) are also included for your use. Two pulse stretchers are provided to accommodate instruments with remote start signals shorter than one second (such as Hewlett Packard GCs).

The computer to which you connect the Model 302 must support USB (it must have at least one USB port—rev 2.0 or higher—and use Windows™ 98, 98SE, ME, 2000, XP or newer).

With your purchase of the Model 302, you should receive the following items:

- 1 - Model 302 Data System box (front and rear views shown below)
- 2 - USB cable for connection to your computer's USB port
- 3 - Manual (either the PeakSimple Chromatography Data Systems or the SRI general product manual)
- 4 - PeakSimple for Windows™ software (inside the manual cover)



The Model 302 comes in a sturdy aluminum box consisting of top and bottom halves, secured together with two brass thumbscrews for easy interior access.



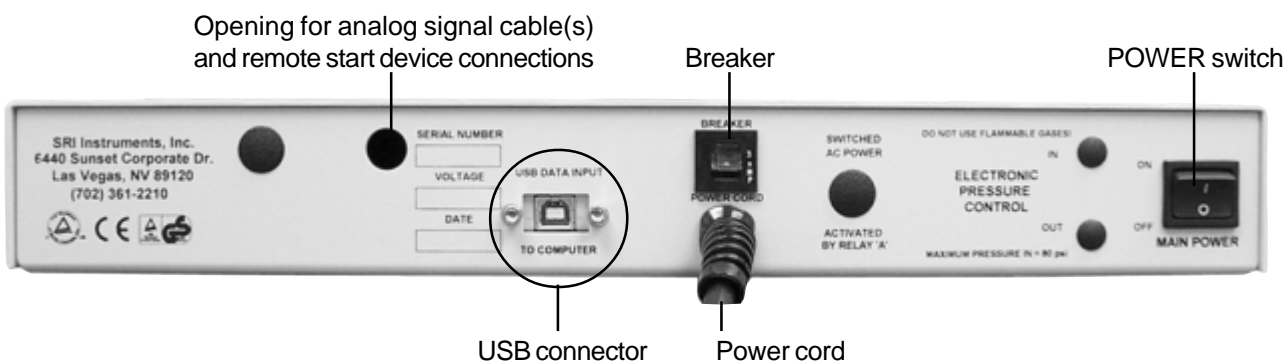
The brass thumbscrews are on the left- and right-hand panels of the Model 302 box.

Front View



POWER Indicator LED

Rear View

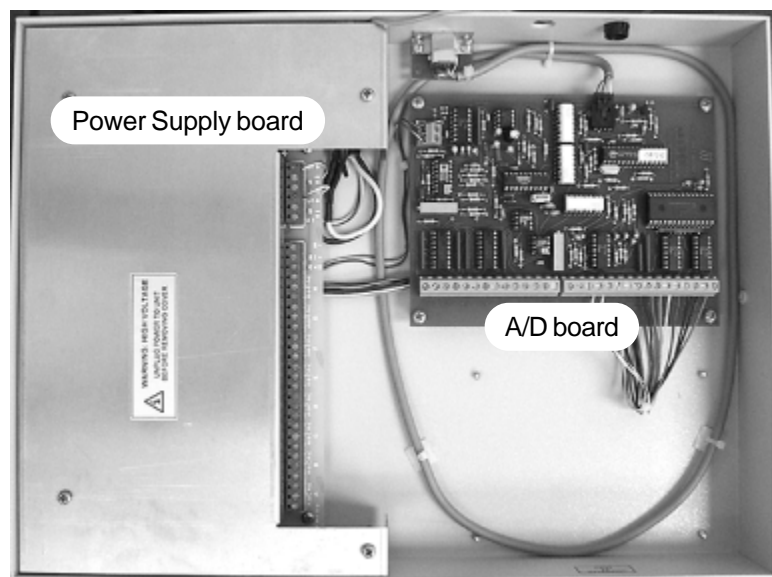


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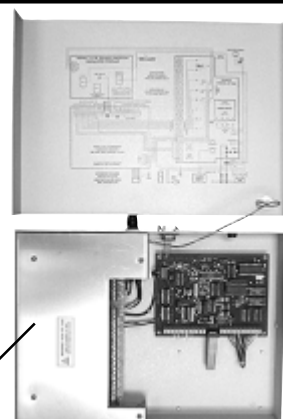
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1. Open the Model 302

Verify that the Model 302 is powered OFF and unplugged. Remove the thumbscrews on both sides of the Model 302 box and slide the top cover up and off. It is connected to the bottom of the box by a ground wire, so just set it next to the bottom half of the box.



High voltage aluminum safety cover

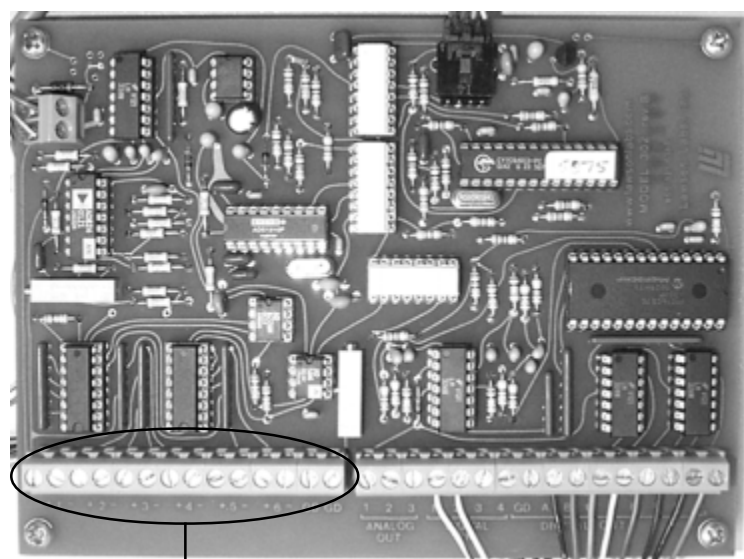


The Model 302 box contains two circuit boards. The board on the right-hand side is the A/D board. The board on the left-hand side under the removable high voltage aluminum safety cover is the Power Supply board. **If you need to remove the high voltage aluminum safety cover, ALWAYS unplug the Model 302 from the wall power outlet first** (you do not need to remove it for the wiring connections described here).

2. Connect the Analog Signal Cable(s)

NOTE: The analog output from some GCs and LCs can have a range of up to 10 volts DC. The Model 302 can tolerate this voltage input, but signals above 6 volts will generate unwanted noise and signals above 5 volts will be “clipped” (the tops of the waveforms will be cut off). Use the 1 volt output typically available on the back of your instrument.

2-1. Route the analog signal cables from your instrument through the open hole in the back of the Model 302.



Channels 1-6 and GD (ground) screw terminals

2-2. Strip 1/4” of insulation from the “signal+” and “signal-” wires of your instrument’s signal cables.

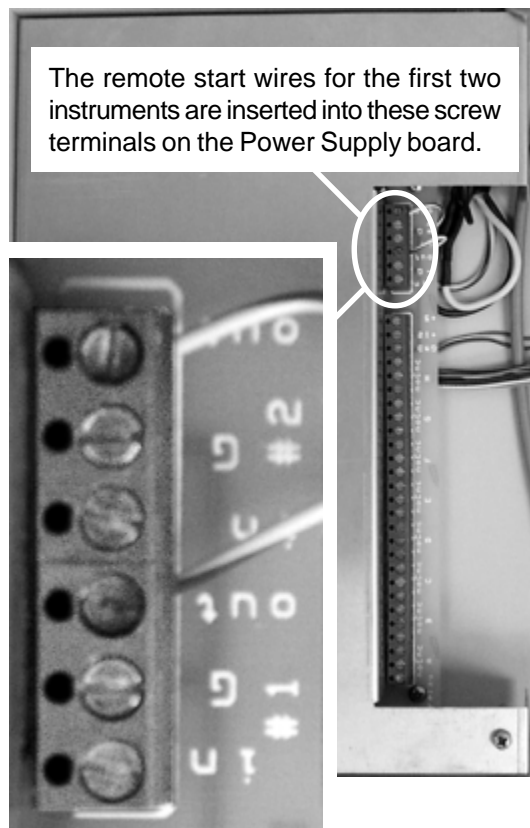
2-3. Remove any jumpers placed in the Channels 1-6 screw terminals at the factory. Insert the “signal+” wire into the A/D board screw terminal marked “1 +” and secure the connection with a small flat-blade screwdriver.

2-4. Insert the “signal-” wire into the A/D board screw terminal marked “1 -” and secure the connection.

2-5. Repeat the connection of signal cables for channels 2, 3, 4, 5, and 6. Any unused channels **MUST** have both inputs jumpered to ground.

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3. Connect the Remote Start Cables (OPTIONAL)

The Model 302 remote start capability allows you to start the data system by means of a switch closure. Four separate remote start circuits permit the user to individually start TIMEBASE 1, 2, 3, and 4 of the data system. In some applications, the chromatograph being used with the Model 302 may offer a remote start signal output or switch closure output that permits starting an integrator or other device when the START button is pressed on the chromatograph's on-board control panel. Typically, this signal can be used to start the Model 302. TIMEBASES 1 and 2 are equipped with pulse stretchers.

3-1. Route the remote start cable from your instrument through the open hole in the back of the Model 302.

3-2. Strip 1/4" of insulation from the "+" and "-" wires of your remote start cable(s).

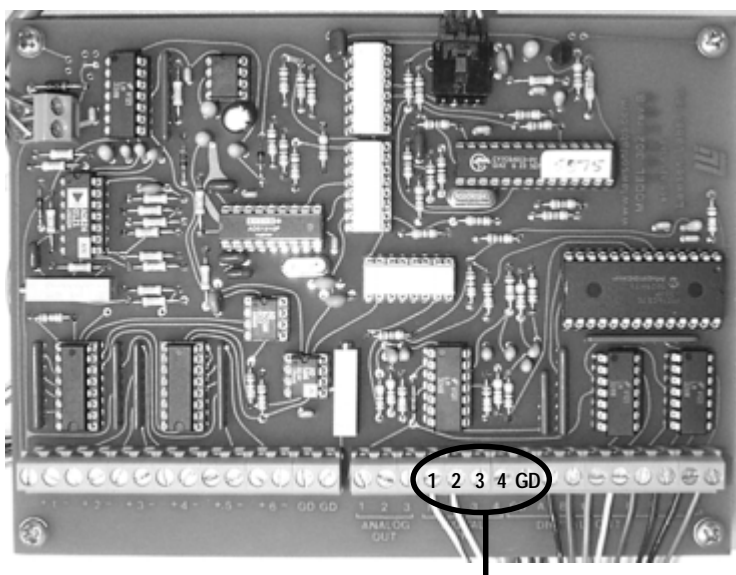
3-3. Insert the "+" wire into the Power Supply board screw terminal marked "#1 IN" and secure the connection.

3-4. Insert the "-" wire into the Power Supply board screw terminal marked "#1 G" and secure the connection.

3-5. For a second instrument, insert the "+" wire into the "#2 IN" terminal, and the "-" wire into the "#2 G" terminal.

3-6. The screw terminals for the third and fourth instruments' remote starts are on the A/D board. The bank of screw terminals is labeled "DIGITAL IN" under "1 2 3 4." Connect the "+" wires for the third and fourth instruments to screw terminals 3 and 4, respectively. Connect both "-" wires to the "GD" screw terminal next to the "4" screw terminal (on the right-hand side).

NOTE: TIMEBASES 3 and 4 require a remote start signal that persists longer for than one second. Check your instruments' specifications (for example, Hewlett Packard GCs produce a very short remote start pulse, so you should connect one of these to TIMEBASE 1 or 2, which are equipped with pulse stretchers).



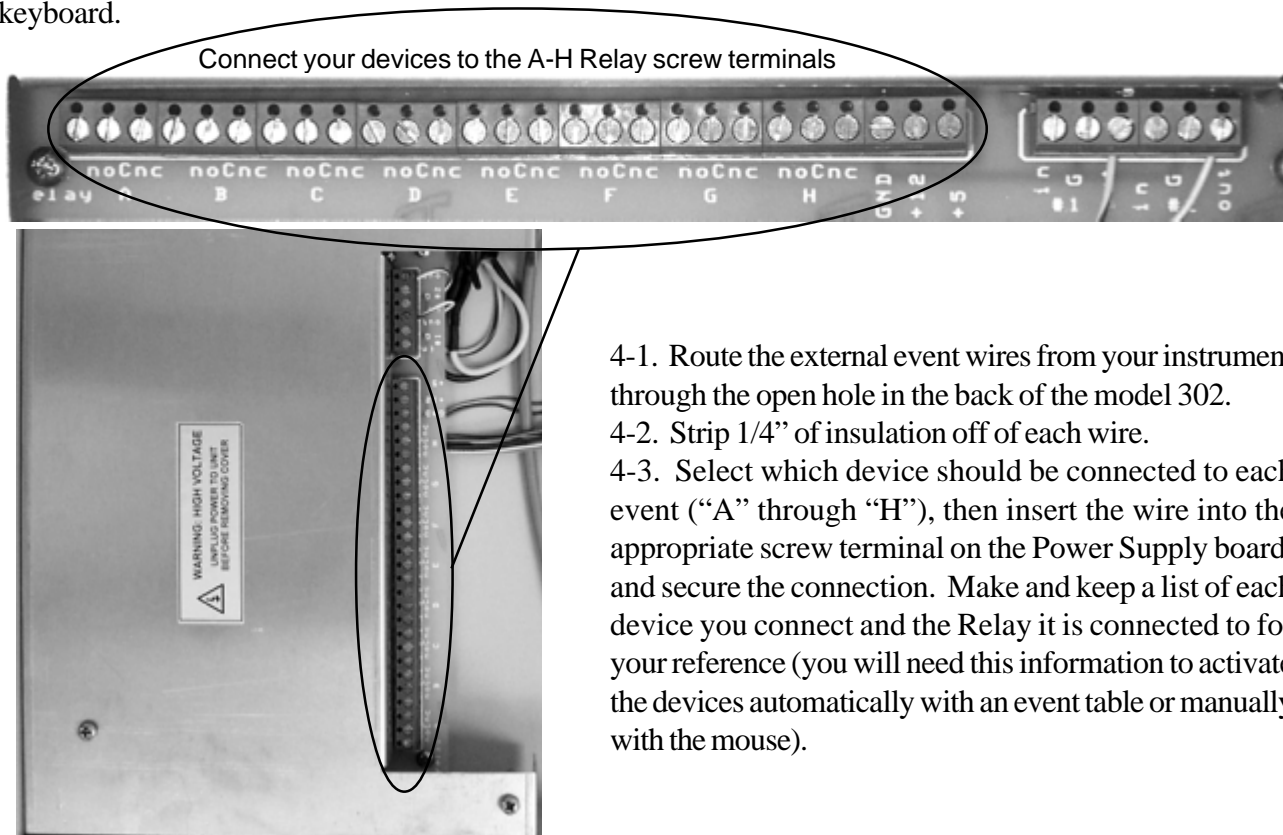
Connect the remote start "+" cables to screw terminals "3" & "4," and the "-" cables to "GD".

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4. Connect the External Event Relay Wires (OPTIONAL)

The Model 302 has eight 0-5 volt TTL level outputs that are wired to a bank of mechanical relays with screw terminals for easy connection to any device which may be operated from a contact closure (normally open [NO] and normally closed [NC] contact closures). These relays may be turned ON and OFF individually and automatically through a PeakSimple timed event table. Manual control is also available via the computer keyboard.

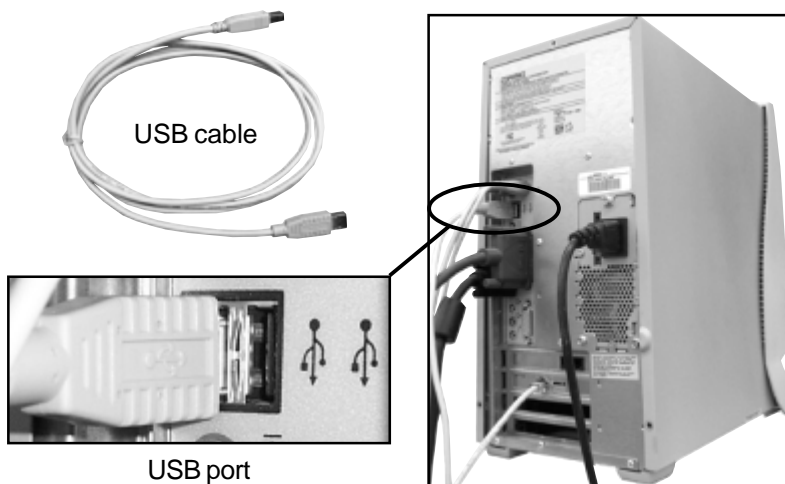


5. Replace the cover on the Model 302 and secure it with the thumbscrews.

6. Connect the USB Cable to Your Computer

The Model 302 is equipped with a USB connector. A USB cable (provided) connects the Model 302 to your Windows™ computer's USB port. This plug and play interface permits the Model 302 to be loaded onto and operated from a desktop or laptop computer that supports USB (rev. 2.0 or higher).

- 6-1. Secure one end of the USB cable to an available USB port on your PC.
- 6-2. Secure the other end to the USB connector on the back of the Model 302.



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7. Connect Power to the Model 302

The Model 302 is provided with a power cord which plugs into a standard 110 (or 220) volt outlet. Plug the Model 302 into the wall outlet. Turn ON the power switch and verify that the POWER LED on the front of the Model 302 is lit.



The power LED is lit when the Model 302 is connected to a power source & switched ON.

8. Install PeakSimple Chromatography Software

8-1. Locate your copy of PeakSimple, which is shipped inside the front cover of your manual. Insert the CD or floppy disk(s) into your computer's appropriate drive.



8-2. Open the appropriate drive through My Computer, then double click on "Setup.exe" and follow the instructions. By default, the setup program places the PeakSimple application directory on the hard drive: c:\peak2000. If you put the application directory elsewhere, take note of the path as you may have to enter it in a dialog box during the USB driver installation procedure.

9. Install the USB Drivers

There are three important files saved to the PeakSimple application directory at the conclusion of the software installation: LL_USB.inf, LL_USB.sys, and LL_USB2K.sys. These files are required for Windows to recognize the A/D board connected to the computer's USB port.

9-1. Double-click on the My Computer icon on your desktop, then on Control Panel, then on Add New Hardware, which should open the Add New Hardware Wizard.

9-2. Click the Next button twice, until you get to the screen that gives you a choice between letting Windows find the new hardware, or selecting it yourself from a list. Click the radio button to choose the hardware from a list and click the Next button.



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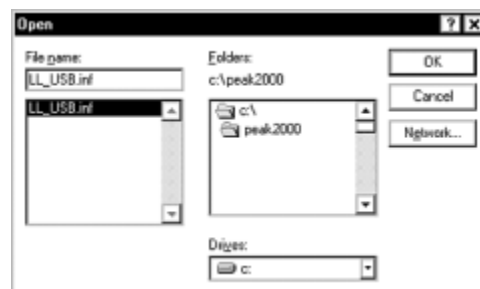
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9-3. Scroll down the hardware list, click on Universal Serial Bus controllers, then click Next. From the following screen click the Have Disk button.



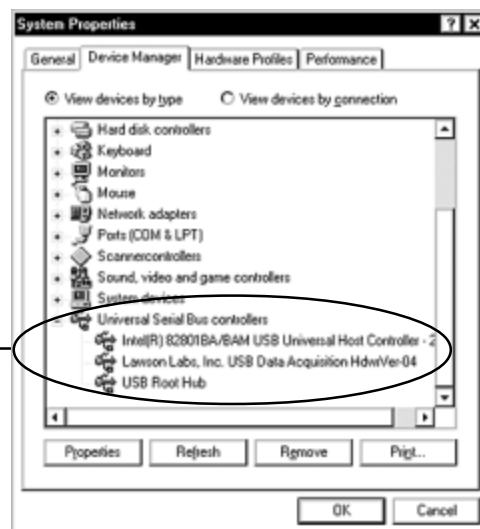
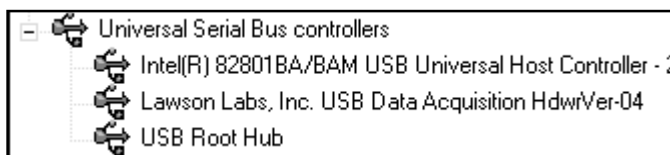
9-4. Click Browse and navigate to the PeakSimple application directory, or type in the path ("c:\peak2000" or the name you have chosen). The Wizard should find the LL_USB.inf file. When you click OK, the Wizard will verify that you want to copy files from the PeakSimple directory ("Copy manufacturer's files from: c:\peak2000").



9-5. When you click OK again, the Wizard will confirm that the drivers are for Lawson Labs. Click Next on this screen and the following screen, and Windows will finish installing the software for the Model 302. Click Finish.



9-6. Restart your computer (you MUST restart your computer before the drivers will work). Open the Control Panel again, then System, then click on the Device Manager tab. If the USB drivers have been successfully installed, the Universal Serial Bus controllers section will list "Lawson Labs, Inc. USB Data Acquisition HdwrVer-04."




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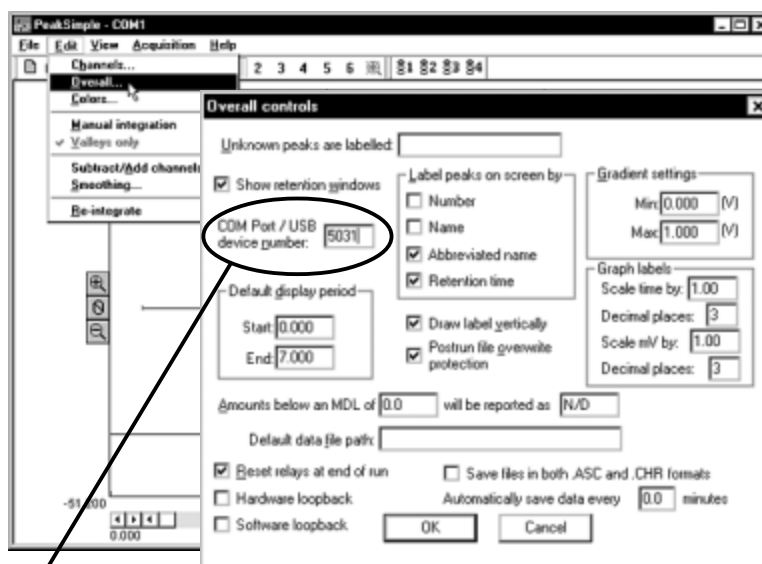
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10. Launch PeakSimple

10-1. Double-click on the PeakSimple icon to launch the program. Verify that communication has been established between your computer and the Model 302. An error message will appear if communication is not established. This is normal until you complete the following step.

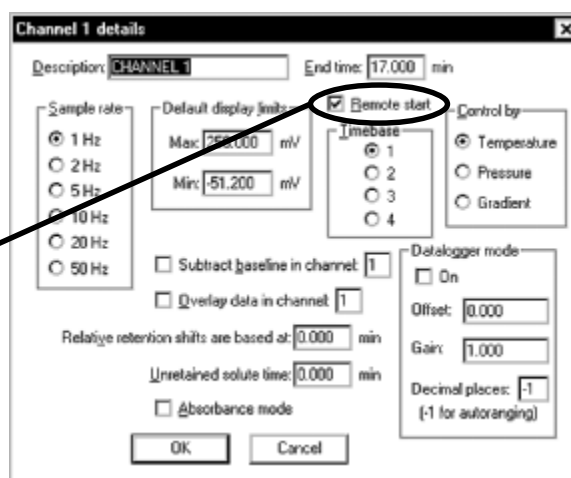


10-2. Each SRI USB data system has a unique 4-digit USB device number beginning with “5” (5031, 5032, etc.). This I.D. number is printed on the back of your Model 302, and on your PeakSimple disk. Open the PeakSimple Edit menu and choose Overall. Enter your Model 302 I.D. number in the box labeled “Com port / USB device number.” Click OK, and PeakSimple will attempt to “wake-up” the data system. Click the Save All  icon so you don’t have to re-enter the USB device number.



Enter the 4-digit USB device number here

10-3. For the remote start option:
Open the Edit menu and choose Channels. Click on the Details button for channel 1. Verify that Remote start is enabled (the box should be checked). Repeat this step for channels 2-6 if necessary.



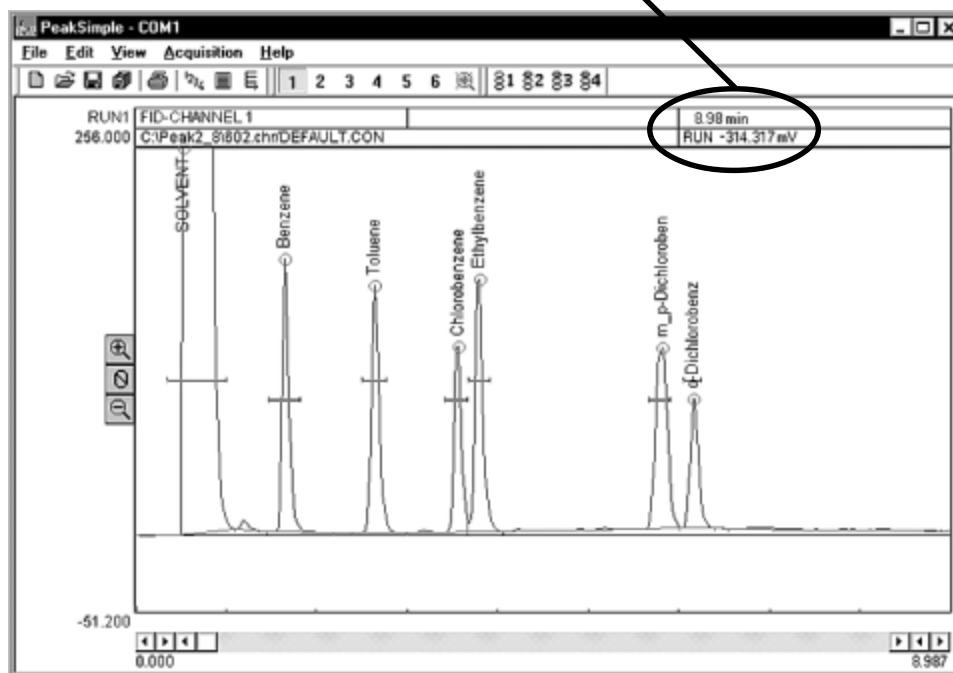
10-4. For information about using Event tables, manual Relay activation, etc., see the “PeakSimple Tutorials” and the “PeakSimple Software” sections in the manual (and online at www.srigc.com—click on the “Download Our Documents” button on the homepage).

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11. Starting an Analysis

10-1. The upper right corner of the PeakSimple chromatogram window contains real-time information pertinent to your analysis in progress. The status of the run (STAND BY, RUN) is displayed in capital letters next to the millivolt (mV) reading, underneath the amount of time into the run.



11-2. Hit your computer keyboard spacebar to begin the run, and the data is plotted onscreen in the chromatogram window.



Press the spacebar to begin the run

Press the End key to stop the run

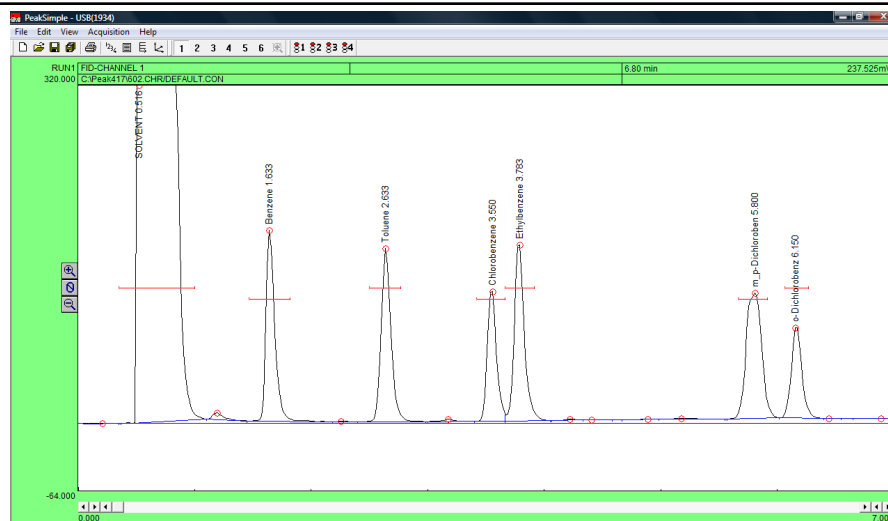
11-3. Hit the End key on your computer keyboard to stop the run.

Technical Support:

If you have questions or problems, call SRI for free technical support at 310-214-5092, 8am - 5pm California time.

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Installing PeakSimple from the CD or USB thumb drive:

- Start the Windows operating system in use on your computer. (Windows XP, Vista, or 7)
- Insert the CD or USB thumb drive into the computer.
- Open **My Computer** and open either the CD or thumb drive.
- Double-click on the **Setup.exe** file. Make sure to select the right version of PeakSimple to install (32- or 64-bit). Windows XP and some Vista computers need to install the 32-bit version, other Vista computers and Windows 7 need to install the 64-bit version. If you are unsure, right-click on **My Computer** then select **Properties** in order to determine what bit operating system you are using.
- To complete installation follow the onscreen instructions provided by the installation wizard.
- For instructions on loading the driver, please refer to the Quick Start Documents located in the PeakSimple folder or on the www.srigc.com website.

Installing PeakSimple from software download:

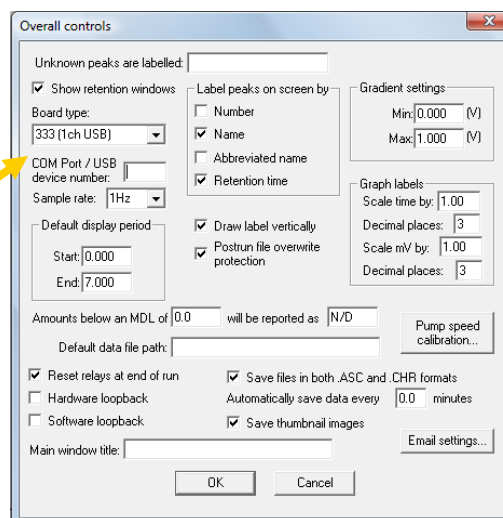
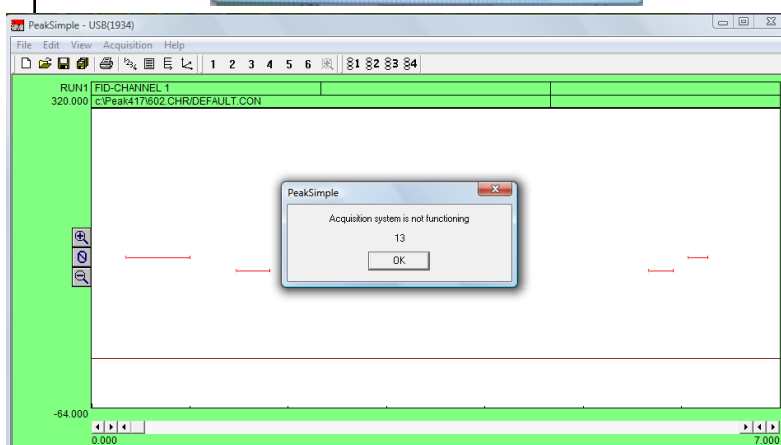
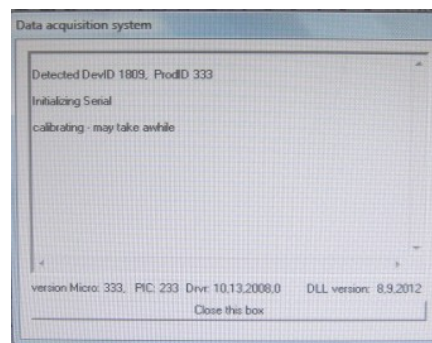
- Start the Windows operating system and use an online browser to access www.srigc.com.
- From the menu on the left hand side of the screen select **Download PeakSimple** and then download the latest version. Windows XP and some Vista computers need to download the 32-bit version, other Vista computers and Windows 7 need to download the 64-bit version. If you are unsure, right-click on **My Computer** then select **Properties** in order to determine what bit operating system you are using.
- Save the file to a temporary folder and double-click on the setup file when it is finished downloading, or, just click **Run** to install PeakSimple without saving the setup file.
- Follow the onscreen instructions provided by the installation wizard.
- For instructions on loading the driver, please refer to the Quick Start Document located in the PeakSimple folder or on the www.srigc.com website.

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Launching PeakSimple

1. Double-click on the Desktop PeakSimple icon to launch PeakSimple.
2. The data acquisition system will attempt to initiate communications between the computer and the data 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. The first time PeakSimple connects to a GC or data system open the **Edit** menu and select **Overall** to get to the **Overall Controls** Screen.
5. Enter the proper **Board type** (202, 203, 302, or 333) and **COM Port/USB device number** (Found on data system or GC). Select OK and PeakSimple will establish communications with the data system.
6. 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.



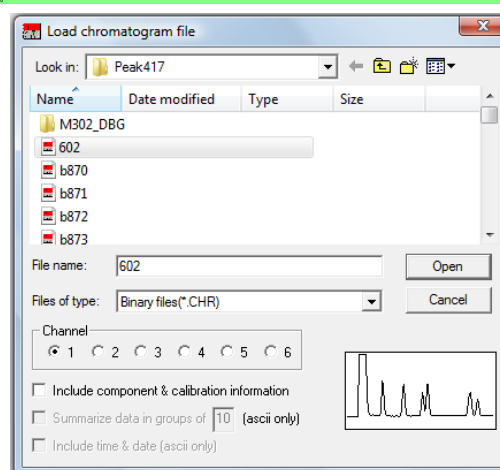
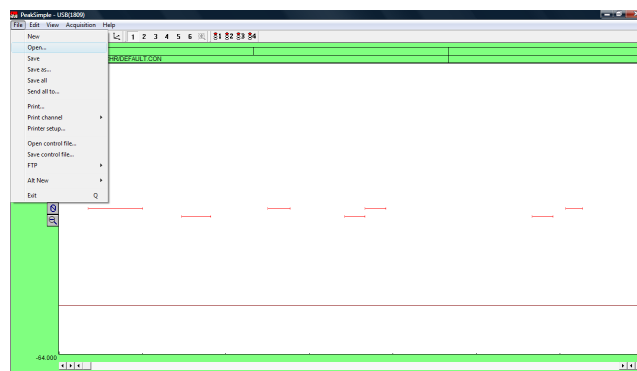
Enter the A/D board type. Your choices are Model 203 single channel serial connection, Model 202 4 channel serial connection, Model 333 single channel USB and Model 302 6 channel USB.

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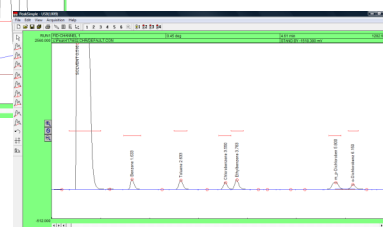
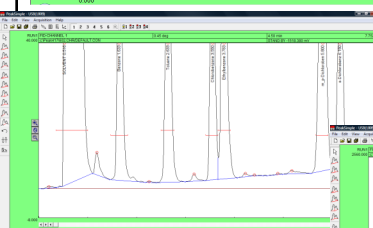
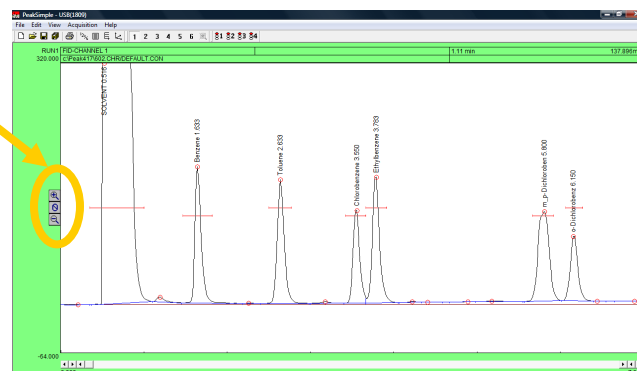
Opening a PeakSimple Data File

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.

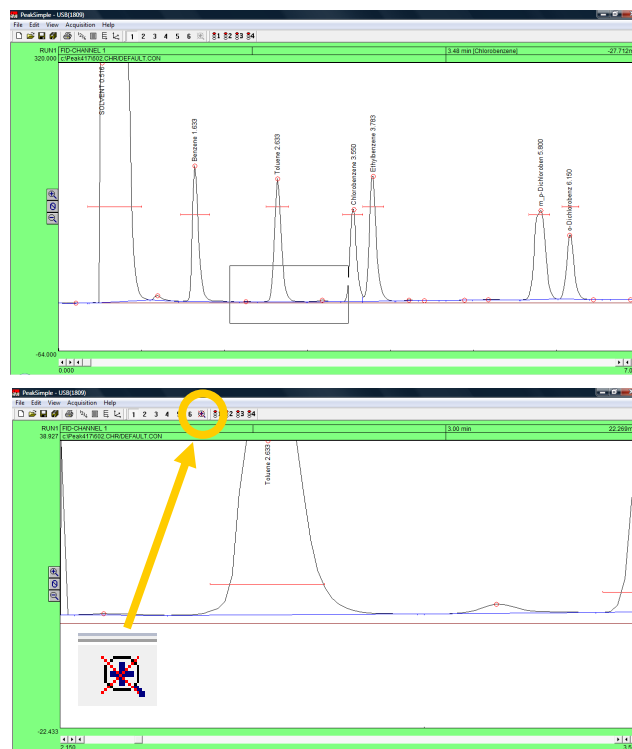


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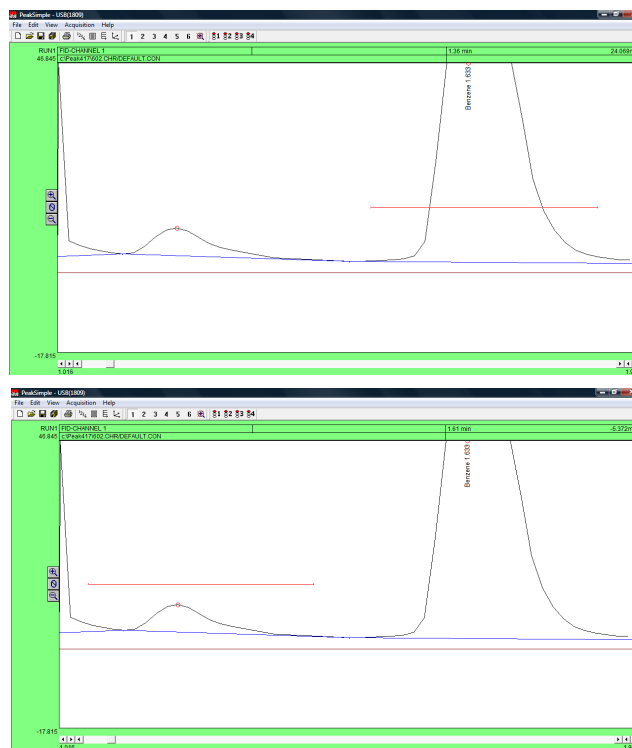
Zooming

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 or right-click and select **Unzoom**.



Dragging Retention Windows

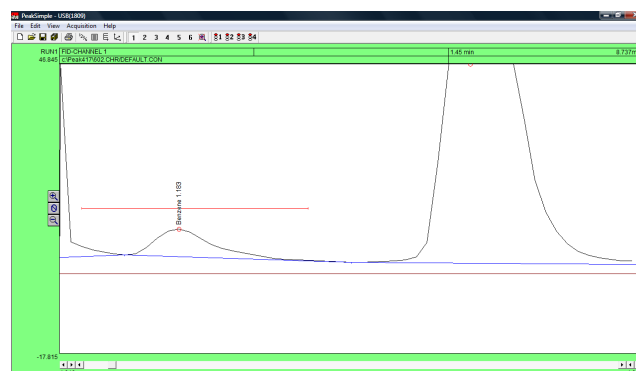
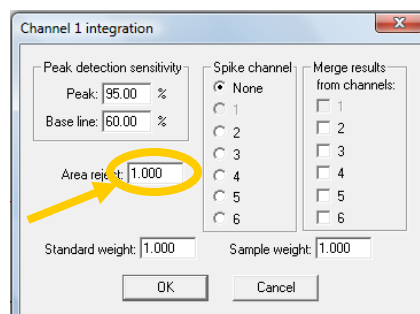
1. To drag a retention window bar place the mouse cursor on the bar until a double sided arrow pops up. Click on the left mouse button and hold and then drag the retention window bar to its desired place.
2. After opening the chromatogram 602.CHR zoom in on the benzene peak and the smaller peak to its 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.



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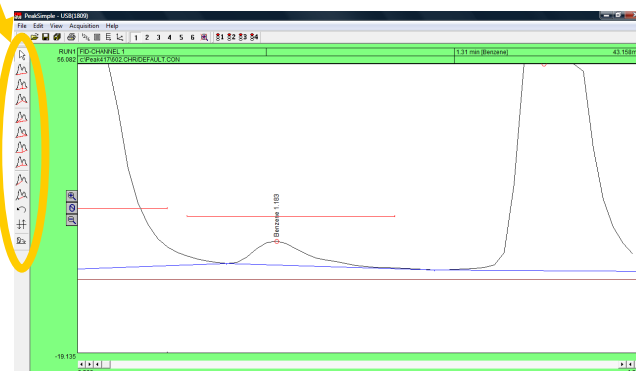
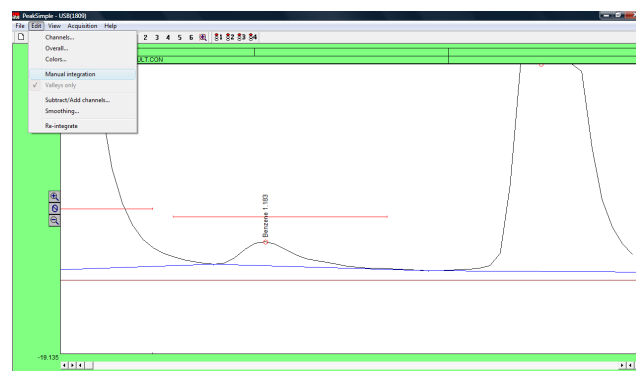
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- Right click on the chromatogram over the unnamed peak and select **Integration** from the resulting menu.
- From the integration window locate the **Area Reject** dialogue box, erase the 100.0 in the box, and add the number **1.0** to the dialogue box. Click **OK** and the integration window will exit.
- Press the **Enter** or **Return** key on your keyboard and the smaller peak will now be recognized as Benzene.



Manual Integration

- 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.
- 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.



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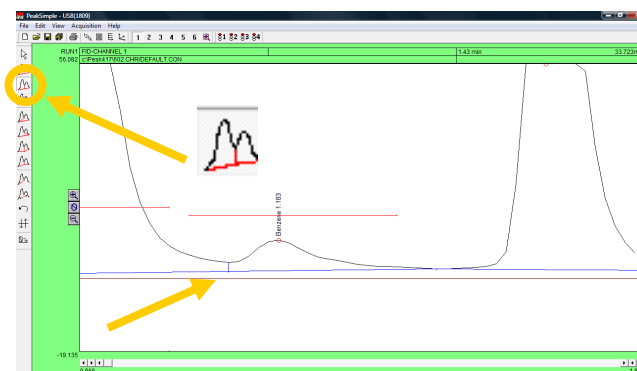
3. To make a baseline “ignore” a peak use the **None** integration tool. After opening chromatogram 602.CHR and the manual integration toolbar, zoom in on the baseline of the solvent peak and the smaller unrecognized peak immediately to its right. Click on the **None** integration tool in the manual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



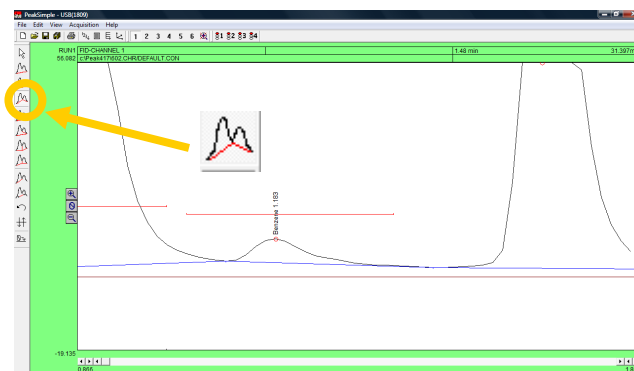
5. Click on the **Undo** tool with your mouse cursor and select the **Drop** integration tool to enable the dropping of the baseline below the two peaks. After selecting the Drop tool click where the valley of the peaks meet the baseline with the cursor. The baseline should now be dropped below the base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



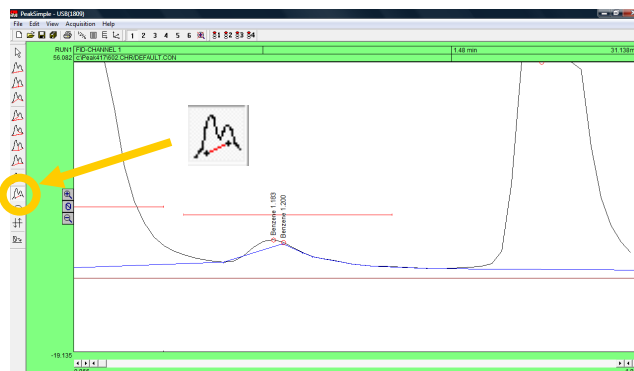
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6. After the manual integration between the two peaks is dropped use the **Based** integration tool to raise the baseline to the valley between the peaks. Once the Based integration tool is selected, click on the valley between the solvent peak and the smaller peak to its right with the mouse cursor. The baseline will now extend up to meet the valley of the two peaks.

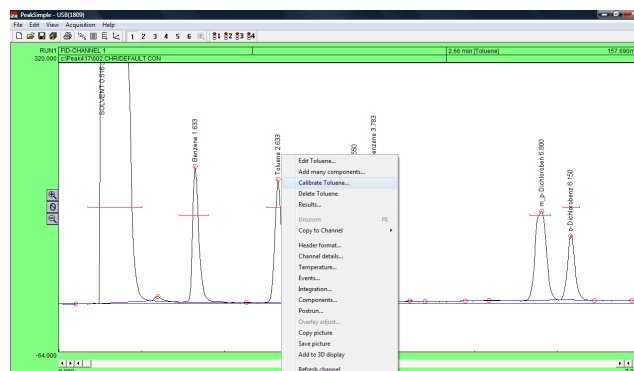


7. Once again click on the **Undo** tool in the manual integration toolbar to remove all changes done to the chromatogram. Select the **Rubber Band** integration tool to manually draw a baseline. Once the Rubber Band tool is selected take the mouse cursor and click on a part of the baseline. While holding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

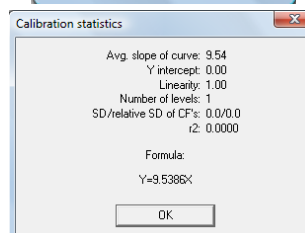
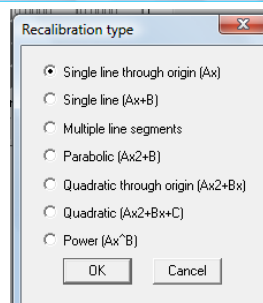
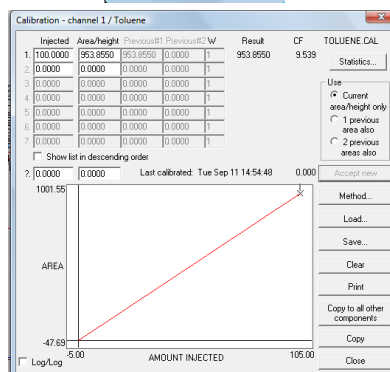
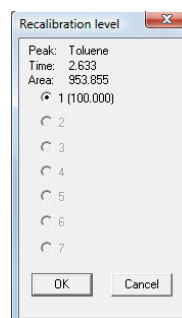
1. To turn the raw area of a peak into a real-world number the peak first needs to be calibrated. To calibrate the Toluene peak in chromatogram 602.CHR, open up the file and then right click using the mouse on the Toluene peak. After right clicking on Toluene select **Calibrate Toluene** from the resulting menu.



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- From the Recalibration level window click on the first level radio button **1 (100.000)** and then select **OK** with your mouse cursor.
- 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 1 and then click on the **Accept New** button to the right of the window.
- Once the new data is accepted, click on the **Method** button immediately below the Accept New button. The Recalibration type window will now open allowing the user to select a method of calibration. By default the calibration type is set at Multiple Line Segments. Select the **Single line through origin (Ax)** radio button and then click on **OK** with the mouse cursor.
- After changing the method of calibration click on **Statistics** in the upper right hand corner of the Calibration level window. The Calibration statistics window will pop up revealing the statistics for the calibration of Toluene. Click **OK** with the mouse cursor to close the Calibration statistics window and then select **Close** from the Calibration window to finish calibrating Toluene.
- View the calibrated results in the Results screen by right-clicking on the chromatogram and selecting **Results**.



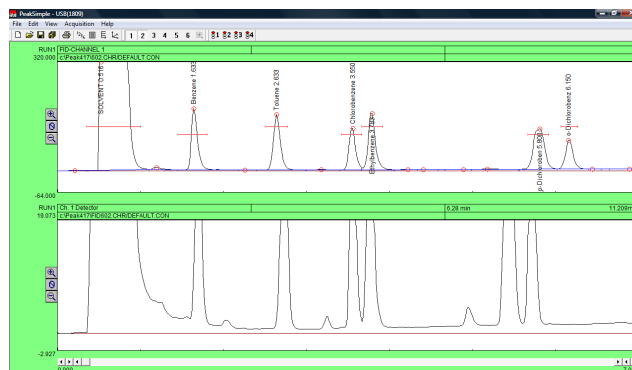
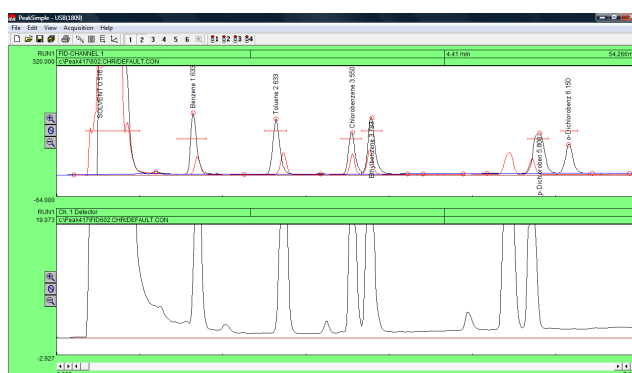
Component	Retention	Area	Height	External	Units
SOLVENT	0.016	71603.5420	888.161	0.0000	%
Benzene	1.633	538.6270	180.764	100.0000	ppm
Toluene	2.633	953.8550	163.086	100.0000	ppm
Chlorobenzene	3.580	676.9720	122.832	72.1215	ppm
Ethylbenzene	3.763	986.4475	166.671	112.3559	ppm
m,p-Dichloroben	5.800	1093.8760	119.019	124.2345	ppm
o-Dichloroben	6.150	537.4520	85.187	54.6115	ppm
		76803.7715		953.3434	

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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 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 black while FID602.CHR is in red.

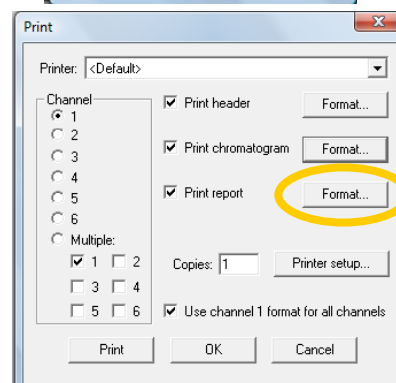
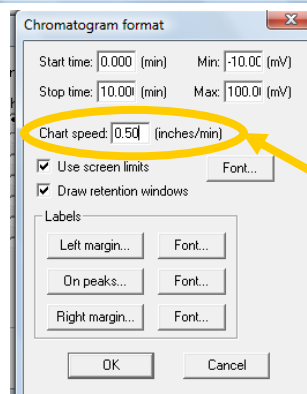
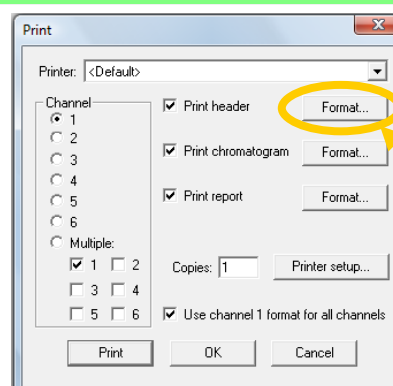
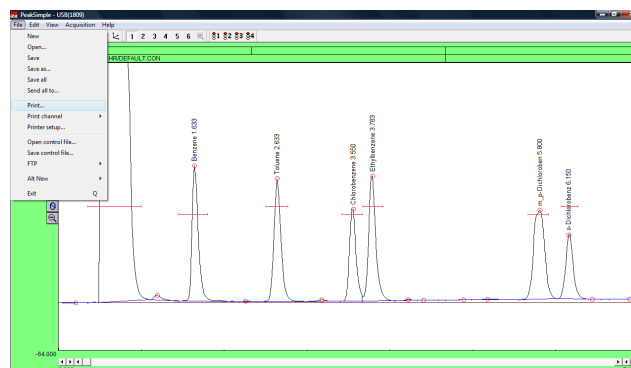



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Printing a Chromatogram

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.

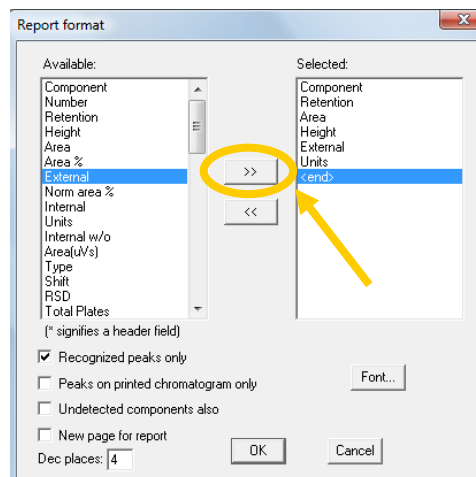


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5. Once the Report format window is open click on **External** in the Available dialogue menu (on the left) and then click with the mouse cursor on the right facing arrow button to add External to the Selected dialogue box (on the right). After External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

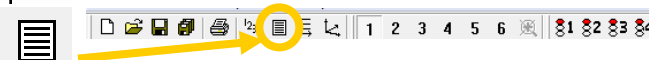
>>



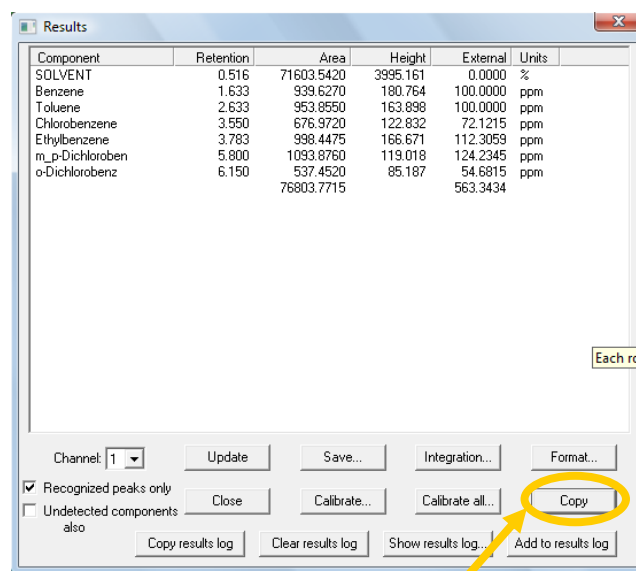
6. Select **Print** in the Print window to print the chromatogram or click on **OK** in the Print window to exit the window.

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.



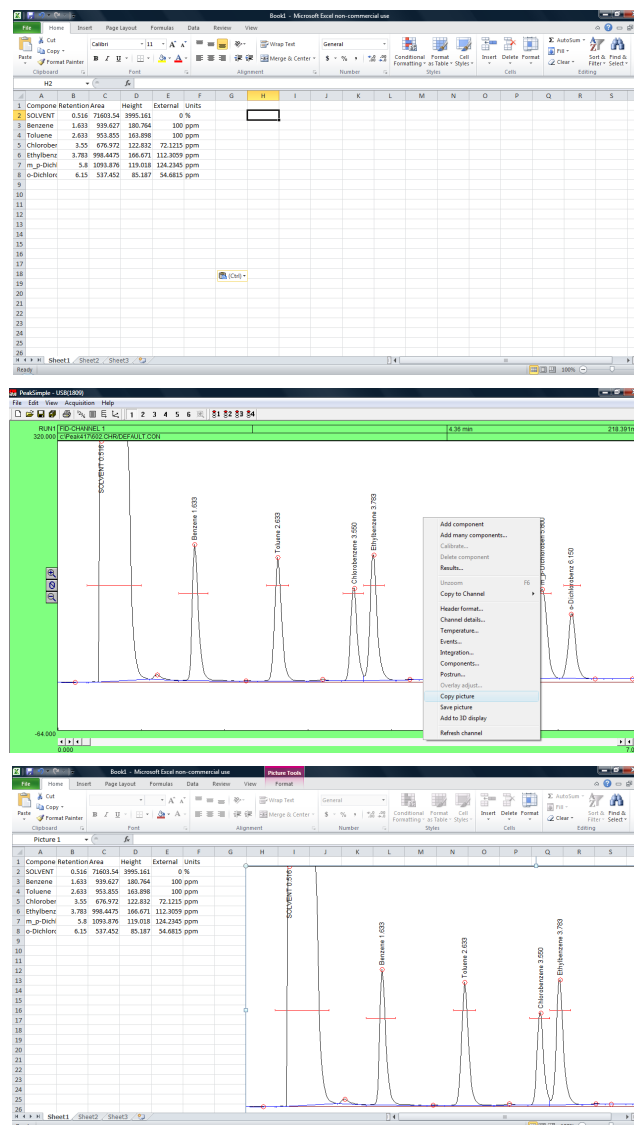
2. Make sure Microsoft Excel is loaded on the computer. If Excel is not loaded you can copy results data and chromatograms to Microsoft Word or PowerPoint. Open up Microsoft Excel by clicking with the mouse cursor on the **Start** button in the bottom left of the Windows screen and then **Programs**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



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- 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 program and hit **Close** to exit the Results window.
- 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.



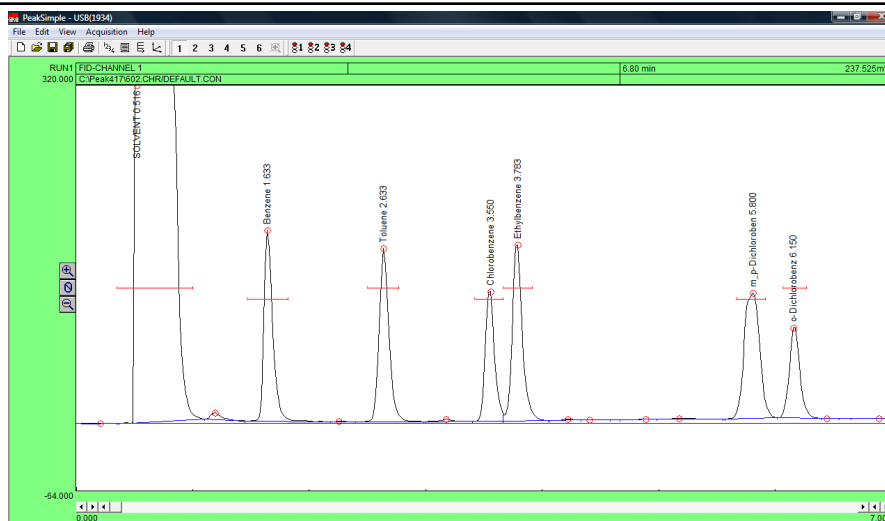
This concludes the PeakSimple Basic Tutorial.

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

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

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Installing PeakSimple from the CD or USB thumb drive:

- Start the Windows operating system in use on your computer. (Windows XP, Vista, or 7)
- Insert the CD or USB thumb drive into the computer.
- Open **My Computer** and open either the CD or thumb drive.
- Double-click on the **Setup.exe** file. Make sure to select the right version of PeakSimple to install (32- or 64-bit). Windows XP and some Vista computers need to install the 32-bit version, other Vista computers and Windows 7 need to install the 64-bit version. If you are unsure, right-click on **My Computer** then select **Properties** in order to determine what bit operating system you are using.
- To complete installation follow the onscreen instructions provided by the installation wizard.
- For instructions on loading the driver, please refer to the Quick Start Documents located in the PeakSimple folder or on the www.srigc.com website.

Installing PeakSimple from software download:

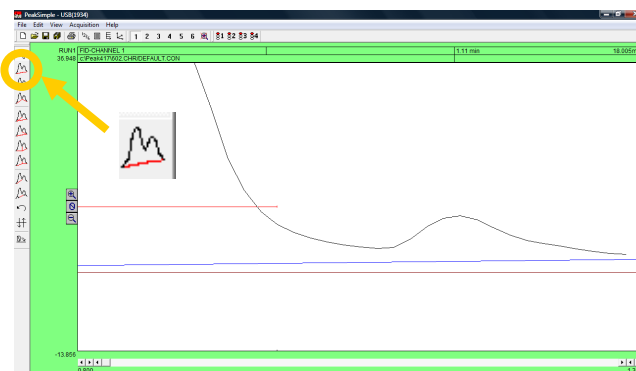
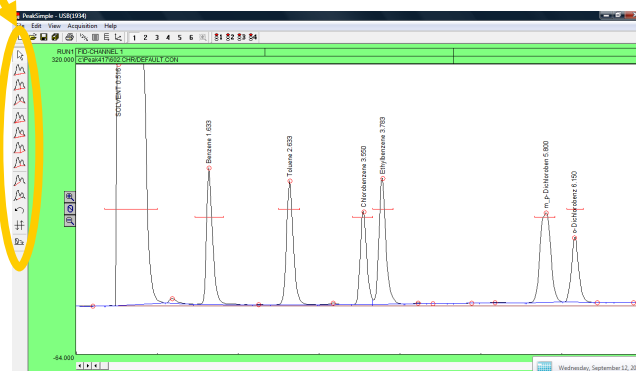
- Start the Windows operating system and use an online browser to access www.srigc.com.
- From the menu on the left hand side of the screen select **Download PeakSimple** and then download the latest version. Windows XP and some Vista computers need to download the 32-bit version, other Vista computers and Windows 7 need to download the 64-bit version. If you are unsure, right-click on **My Computer** then select **Properties** in order to determine what bit operating system you are using.
- Save the file to a temporary folder and double-click on the setup file when it is finished downloading, or, just click **Run** to install PeakSimple without saving the setup file.
- Follow the onscreen instructions provided by the installation wizard.
- For instructions on loading the driver, please refer to the Quick Start Document located in the PeakSimple folder or on the www.srigc.com website.

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Manual Integration

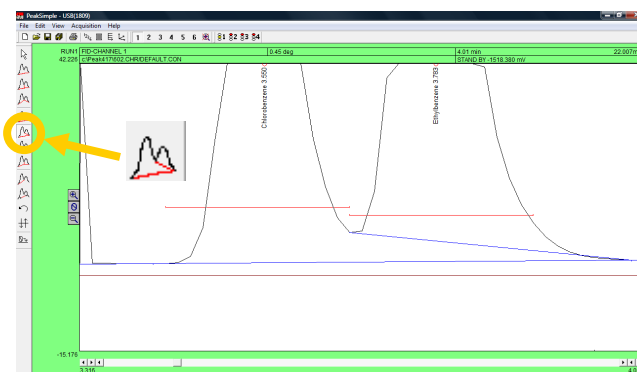
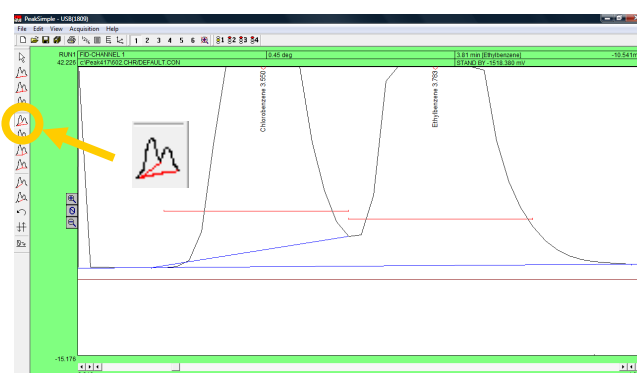
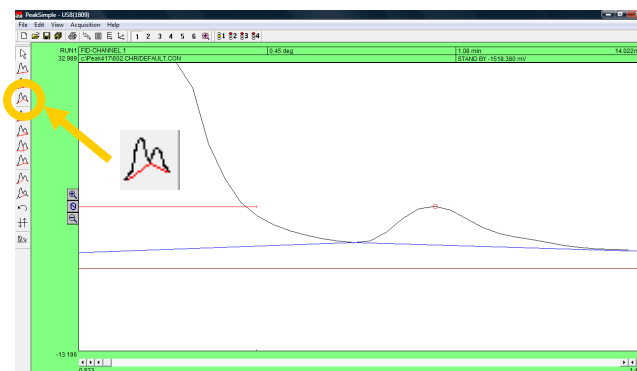
1. To manually integrate the PeakSimple baseline in a chromatogram use the manual integration tools found in the manual integration toolbar. To open the manual integration toolbar first have chromatogram 602.CHR and component file 602.CPT loaded and then select **Edit** from the PeakSimple menu bar. From the drop down menu select **Manual integration** with the mouse cursor. The manual integration toolbar will now be displayed on the left-side of the PeakSimple 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.



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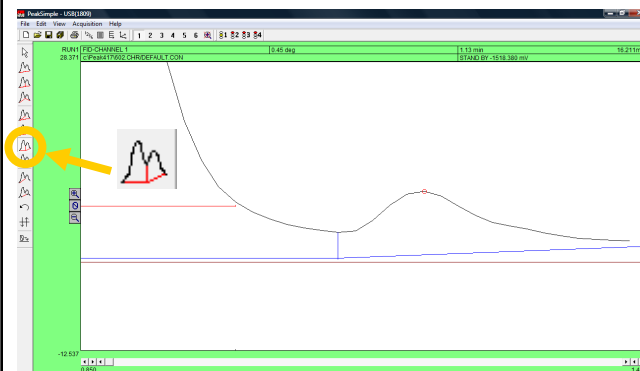
4. The Based integration tool raises the baseline to the valley between two specified peaks. With the baseline dropped, click on the **Based** integration tool button and then click on the valley between the solvent peak and the smaller peak to its right to raise the baseline to the valley.
5. The Lead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



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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.



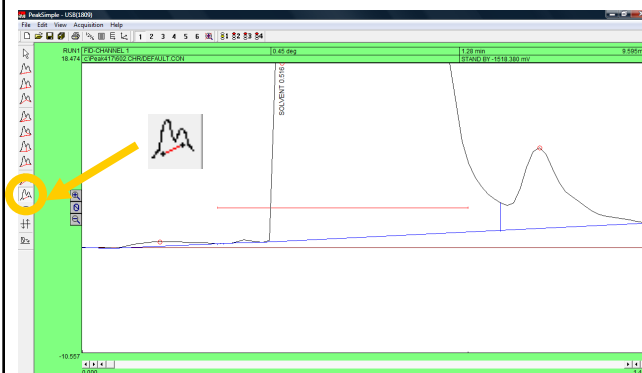
9. The Inhibit tool ends the baseline after a valley effectively inhibiting a peak's area from being counted with the rest of the chromatogram. To use the Inhibit integration tool select the **Inhibit** tool button from the manual integration toolbar and click on the valley of the Solvent peak and the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



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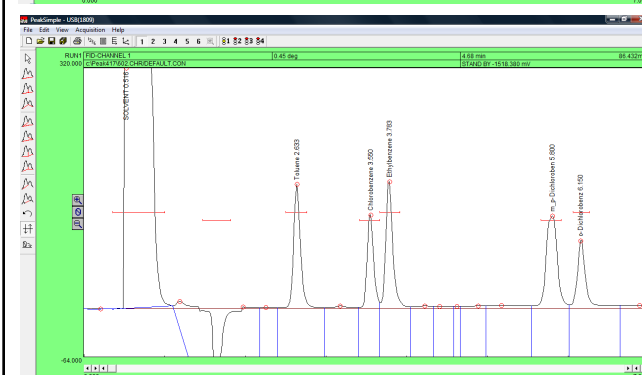
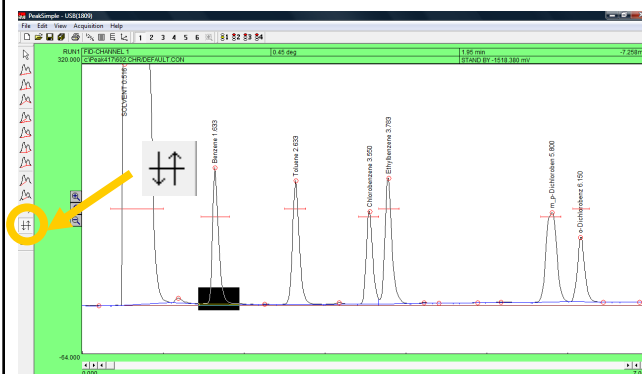
10. The Rubber Band tool is used to manually draw the baseline in a chromatogram. To use the Rubber Band tool first scroll the X-axis scrollbar all the way to the left to **0.000**. Select the **Rubber Band** tool from the manual integration toolbar and draw a line from the valley between the Solvent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



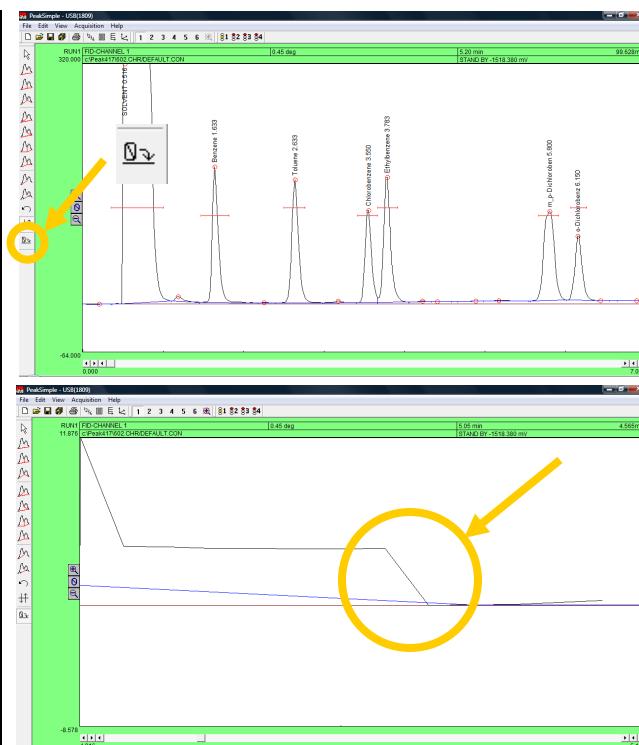
12. The Reverse tool allows the inverting of a peak in a chromatogram. First unzoom off of the Solvent peak and the smaller peak to its right and then select the **Reverse** tool from the manual integration toolbar and click and hold the left mouse button while the area of the chromatogram you want to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



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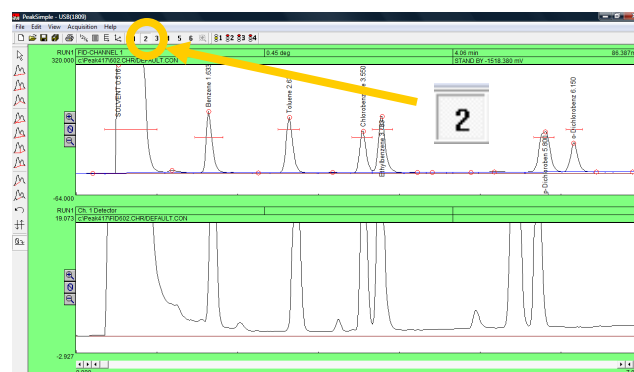
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13. The Zero tool is used to set the value of the data line at a selected point and following in the chromatogram to zero. First undo the changes done to the chromatogram by the Reverse tool by reopening 602.CHR in the PeakSimple menu bar. **Note:** Changes made to a chromatogram by the Reverse tool and the Zero tool cannot be undone with the Undo tool. Once the file is re-opened 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 the Channel 2 radio button and then file **FID602.CHR** from the list of files to open the file in channel 2. Click **OK** with the mouse cursor to load the file.



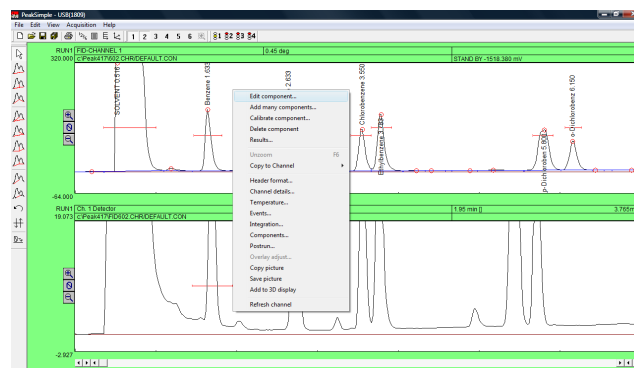
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2. In channel 2 locate the second tall peak from the left and right click on it with the mouse cursor. From the resulting menu select **Add component** to add a retention window bar to the peak. Once again right click on the peak and select **Edit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



Component details

Peak number: 1

Peak name: benzene

Start: 1.47 End: 1.97 Expected: 0.00

Internal standard: 0.000 Units: ppm

Internal standard peak: 0 Ref peak: 0

In case of multiple peaks:

- ☐ Show each peak separately
- ☐ Show first peak only
- ☐ Show last peak only
- ☒ Show largest peak only
- ☐ Show total of all peaks

Measure peak:

- ☒ Area
- ☐ Height

Alarms...

User calculations...

Multiplication factor: 0.00000000

☐ Calculate area as time-slice

OK Cancel

Integrate ☒

Channels

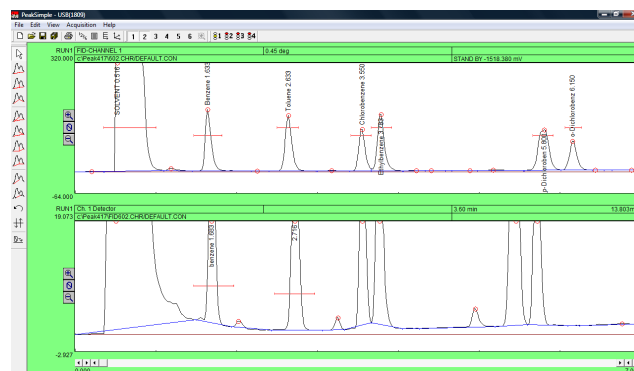
Channel	Active	Display	Integrate	Details	Temperature	Events	Integration	Components	Postrun
Channel 1: FID-CHANNEL 1	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>						
Channel 2: Ch. 1 Detector	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>						
Channel 3: Channel 3	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>						
Channel 4: Channel 4	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>						
Channel 5: Channel 5	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>						
Channel 6: FID-CHANNEL 1	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>						

OK Cancel

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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.



Component details

Peak number: 2

Peak name: toluene

Start: 2.43 End: 2.93 Expected: 0.00

Internal standard: 0.000 Units: ppm

Internal standard peak: 0 Ref peak: 0

In case of multiple peaks:

- ☐ Show each peak separately
- ☐ Show first peak only
- ☐ Show last peak only
- ☒ Show largest peak only
- ☐ Show total of all peaks

Measure peak:

- ☒ Area
- ☐ Height

Alarms...

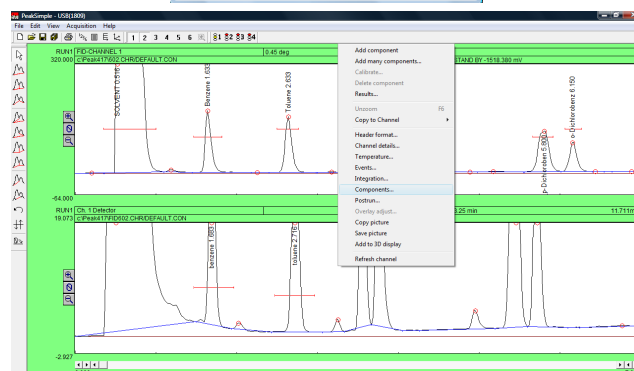
User calculations...

Multiplication factor: 0.00000000

Calculate area as time-slice

OK Cancel

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



Channel 2 components

Ctable.cpt

Peak	Name	Start	End	Calibration
1	benzene	1.470	1.970	
2	toluene	2.480	2.980	

Add... Change... Remove Calibrate...

Load... Save... Clear Print

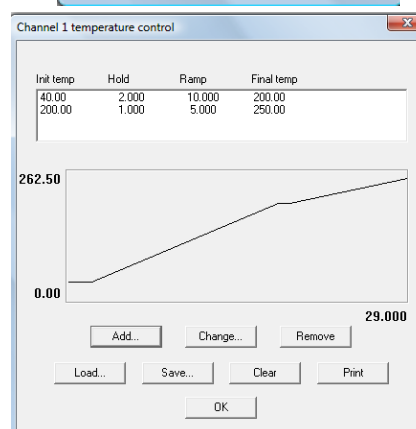
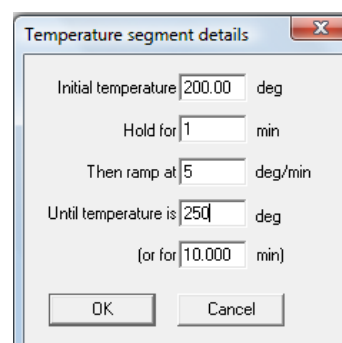
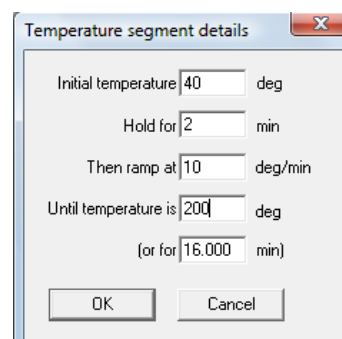
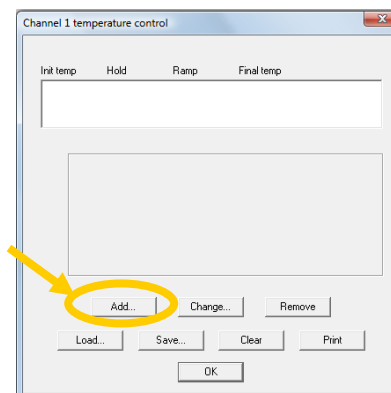
OK

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Temperature Programming

1. To modify the temperature programming in PeakSimple right click anywhere on the chromatogram and choose **Temperature** from the drop down menu. This will open up the Temperature control window.
2. In the Temperature control window select **Add** from the group of buttons. The Temperature segment details window will open allowing the addition or modification of the temperature programming. Enter the numbers shown in the picture to the right in the appropriate fields. 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.

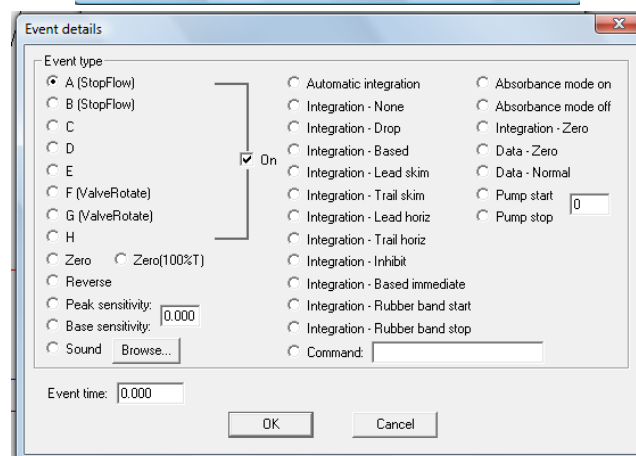
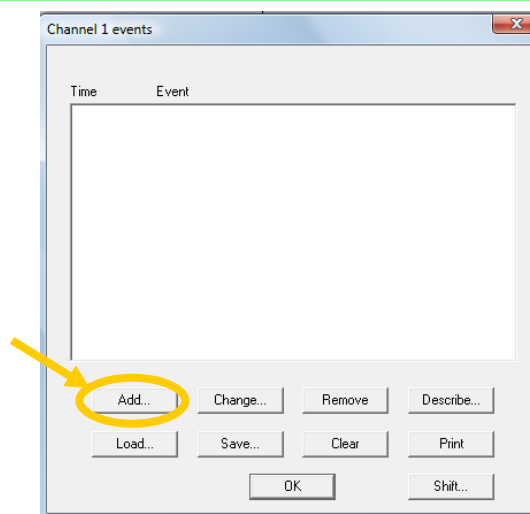
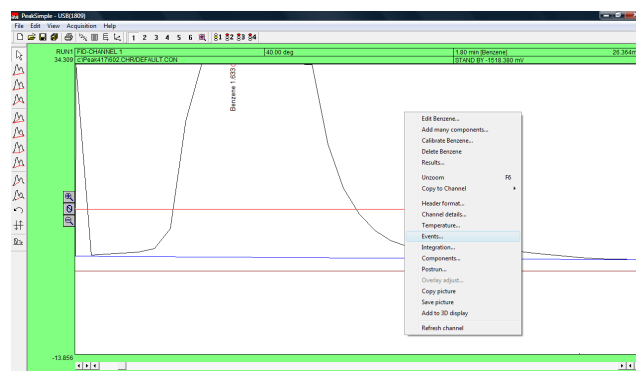


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Events Table

1. To modify 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 A/D 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 **Re-integrate** from the **Edit** menu bar.*

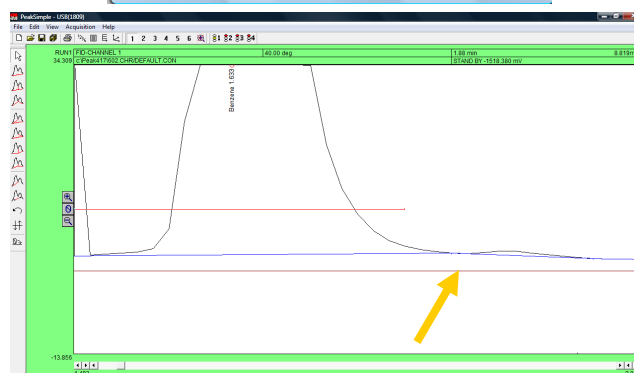
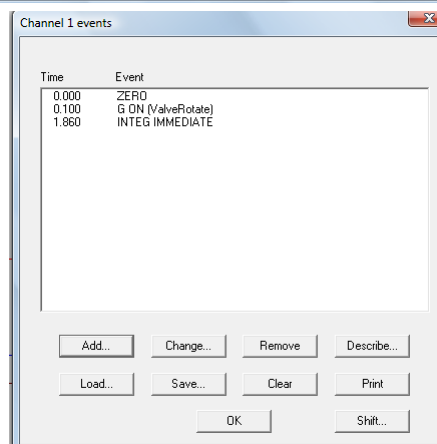
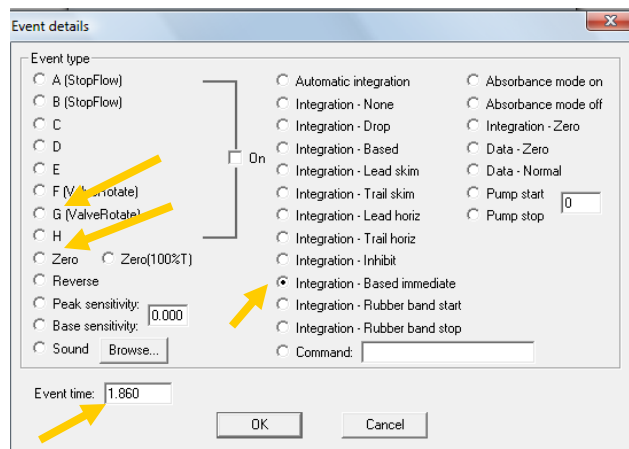


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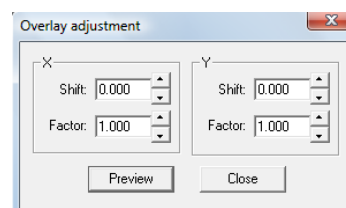
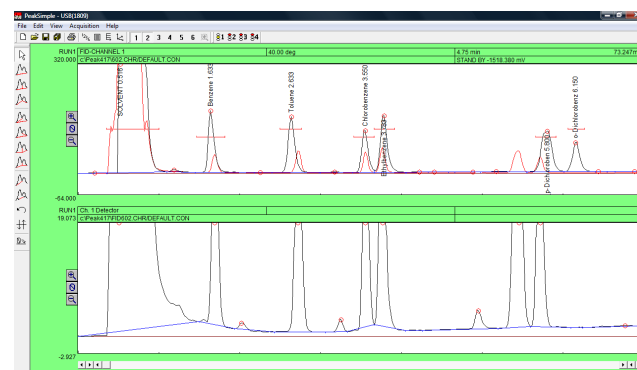
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3. In the Event details window locate and select the relay **G** radio button with the mouse cursor and then locate the Event time dialogue box and enter **.1** in the box. Click on **OK** to exit the window. **Note: The relay might be used to actuate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



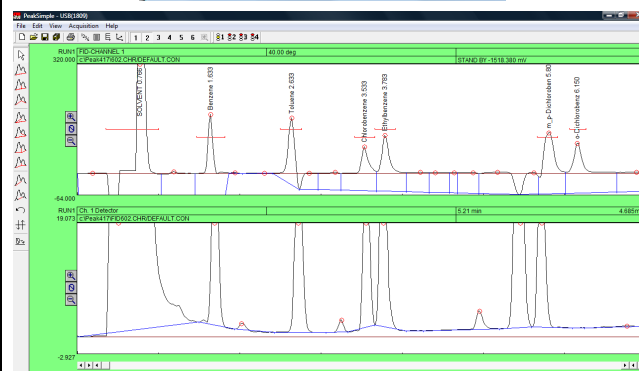
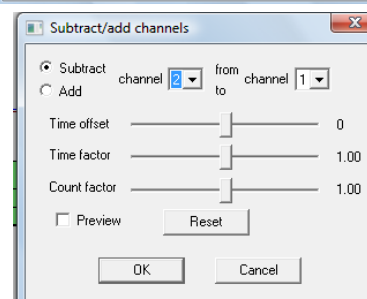
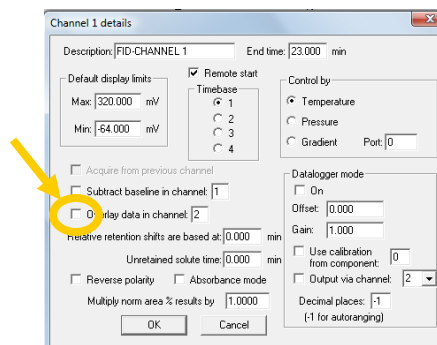
1. To overlay one PeakSimple chromatogram on top of another chromatogram open up a second channel in the main screen and load chromatogram 602.CHR in the first channel and chromatogram FID602.CHR in the second channel. Right click anywhere in the first channel and select **Channel details** from the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



PeakSimple Advanced Tutorial

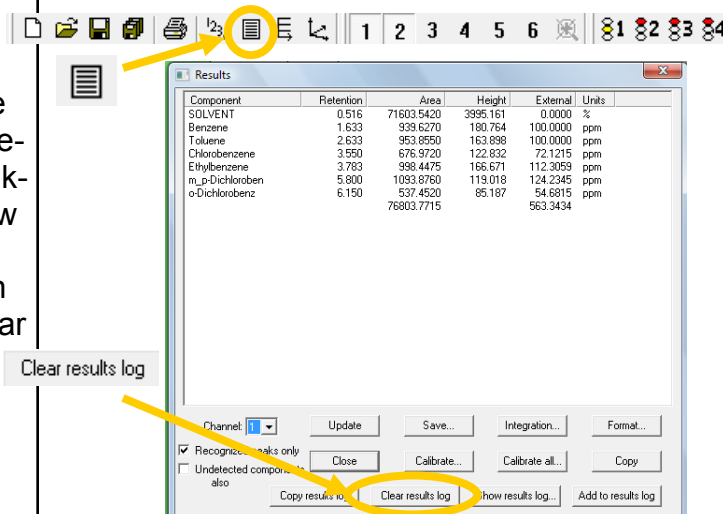
Version 4.17, September 2012

- To subtract a chromatogram in one channel from another channel, right click using the mouse cursor on channel 1 and select **Channel details**. From the Channel 1 details window deselect the Overlay data in channel checkbox and then click on the **OK** button to exit the window.
- Go to the **Edit** menu bar and select **Subtract/Add channels** from the drop down menu. In the Subtract/add channels window make sure the Subtract radio button is selected and that channel 2 is being taken from channel 1. Click on the **OK** button to make the changes take effect and have channel 2 subtracted from channel 1. The normal way to use this feature is to subtract a drifting baseline from a chromatogram.



Results Log

- Open chromatogram 602.CHR in the PeakSimple main screen and then select the **Results** button from the PeakSimple toolbar. In the Results window click on the **Clear results log** button at the bottom of the window. Click on **Yes** from the resulting window to clear the results.



PeakSimple Advanced Tutorial

Version 4.17, September 2012

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.

602.CHR	12/14/1989	14:39:01	'SOLVENT'	0.516	71603.5420	3995.161	0.0000
602.CHR	12/14/1989	14:39:01	'SOLVENT'	0.516	71603.5420	3995.161	0.0000
602.CHR	12/14/1989	14:39:01	'SOLVENT'	0.516	71603.5420	3995.161	0.0000

Copy results log

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	602.CHR	12/14/1989	14:39:01	'SOLVENT'	0.516	71603.54	3995.161	0.0000											
2	602.CHR	12/14/1989	14:39:01	'SOLVENT'	0.516	71603.54	3995.161	0.0000											
3	602.CHR	12/14/1989	14:39:01	'SOLVENT'	0.516	71603.54	3995.161	0.0000											

Channel 1 post-run actions

☒ Save file as: 602.CHR ☒ Auto-increment

☐ Or use list of filenames: List

☐ Save results ☒ Add to results log: CH1.LOG

☐ Print results ☐ Update ODE link ☐ Save picture

Execute: _____

☐ Restart run after: 10.00 minutes 0 times total (0 remaining)

☐ Recalibrate at level: 1 ☐ Save results file to FTP site

☐ Smooth first ☐ Save data file to FTP site

☐ Copy data to channel: 1

☐ Add to 3D display

Email: ☒ No ☐ On alarm condition ☐ Always

OK Cancel

This concludes the PeakSimple Advanced Tutorial

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

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

PeakSimple update tips for serial (non-USB) interfaces

If you are updating to the latest version of PeakSimple software and have a serial interface to your GC or data system then you will have to enter the correct board type in Peaksimple's Edit/Overall screen.

PeakSimple now support four different A/D boards, two serial types and two USB types.

Enter the board type and the comport here in the Edit/Overall screen.

Also enter the comport number in the field immediately below the board type.



This is a serial cable

Overall controls

Unknown peaks are labelled:

☒ Show retention windows

Board type: **202 (4ch serial)**

Start: 0.000
End: 17.000

Label peaks on screen by:
☐ Number
☒ Name
☐ Abbreviated name
☒ Retention time

☒ Draw label vertically
☒ Postrun file overwrite protection

Gradient settings:
 Min: 0.000 (V)
 Max: 1.000 (V)

Graph labels:
 Scale time by: 1.00
 Decimal places: 3
 Scale mV by: 1.00
 Decimal places: 3

Amounts below an MDL of 0.0 will be reported as N/D

Default data file path:

☐ Reset relays at end of run
☐ Hardware loopback
☐ Software loopback

☐ Save files in both .ASC and .CHR formats
 Automatically save data every 0.0 minutes
☒ Save thumbnail images

Main window title:

Pump speed calibration...
 Email settings...

OK Cancel

Copying Data To Excel from PeakSimple

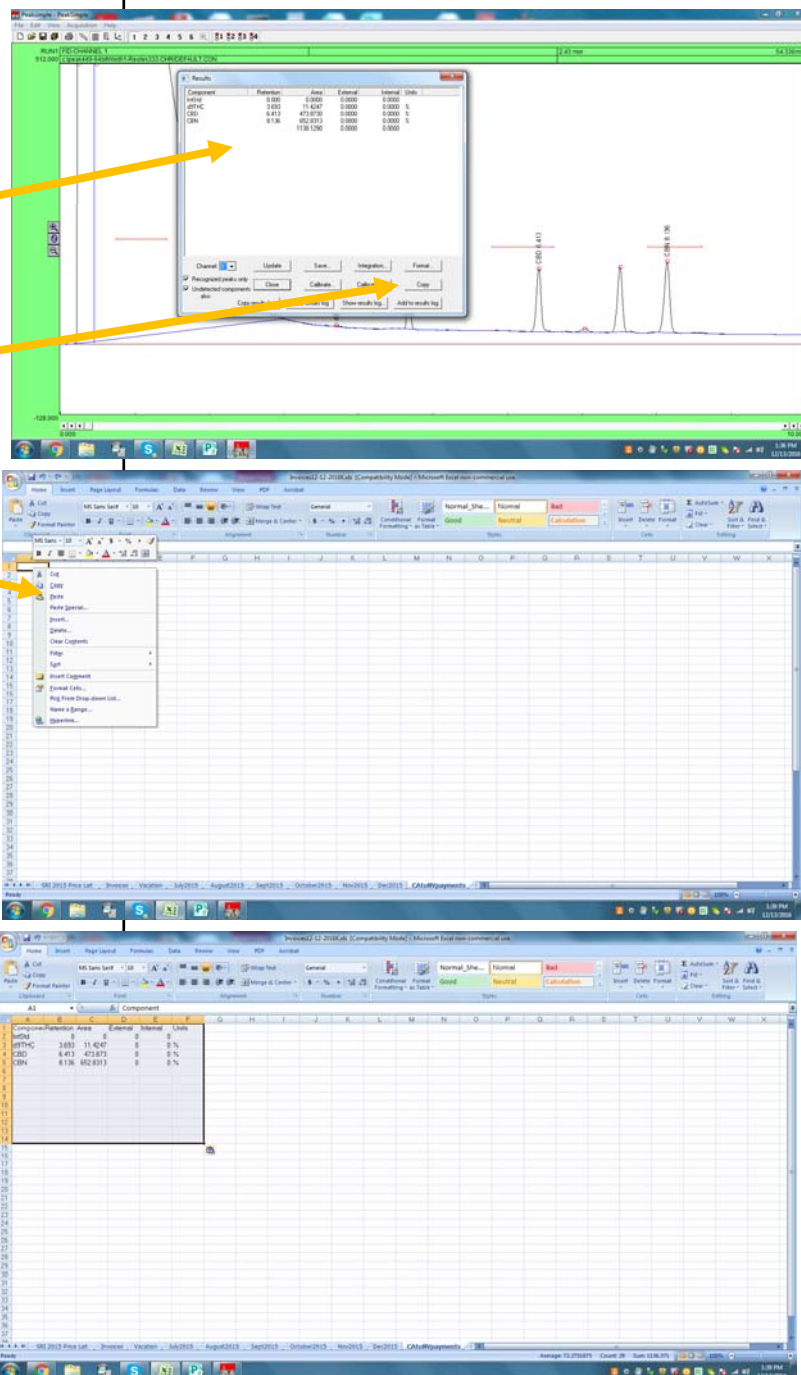
December 2016

The calculated results from the chromatogram on the screen are shown in tabular format in the View/Results screen.

Click the COPY button to copy the results table as a CSV (comma separated variable) file to the Windows clipboard.

From Excel, select a cell, right click and then left click PASTE.

The results table from PeakSimple appears in Excel.



Copying Data to Excel December 2016

Page 1

Copying Data To Excel from PeakSimple

December 2016

Sometimes you want to copy the results of more than one chromatogram into Excel.

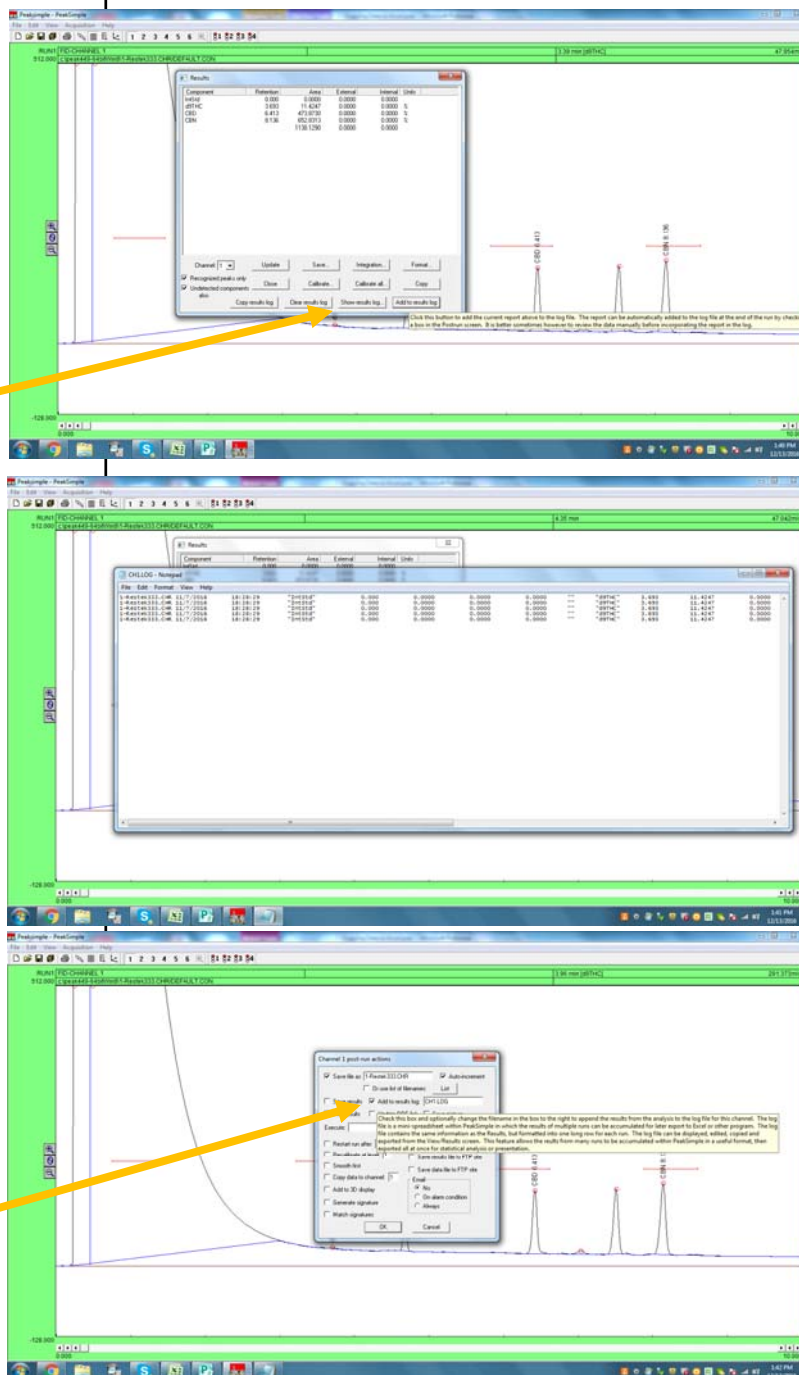
For example, you may be running a series of tests and want to get the results from all the tests into Excel.

Click the button in the Results screen labelled **SHOW RESULTS LOG**.

If there is already a RESULTS LOG it will look something like this. Each line in the results log has a time and date stamp plus the same information as in the results table, except the data is stretched out in one long line for each analysis. Ideally the peak information is perfectly lined up in columns as shown.

If there is not already a results log, then you can add the results table to the log by clicking the button labelled **ADD TO RESULTS LOG** also at the bottom of the Results screen.

The results from each analysis can be added to the results log automatically at the end of each run by checking the box in the Postrun screen labelled **ADD TO RESULTS LOG**. You can also define the name of the results log file. It defaults to CH1.log for channel 1.



Copying Data to Excel December 2016

Page 2

Copying Data To Excel from PeakSimple

December 2016

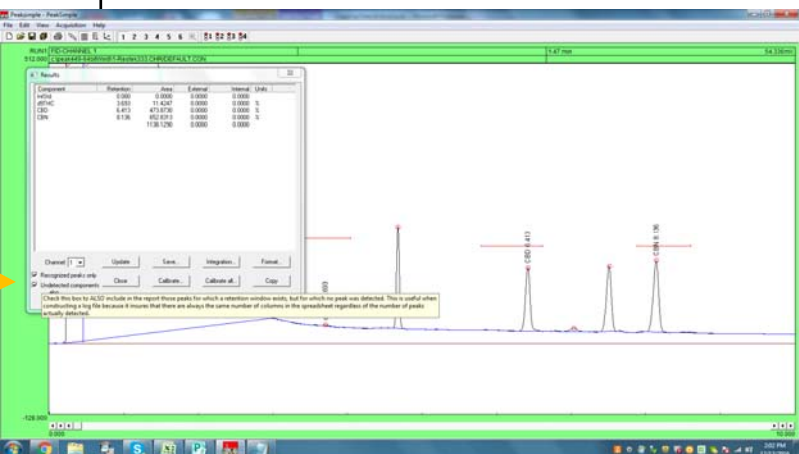
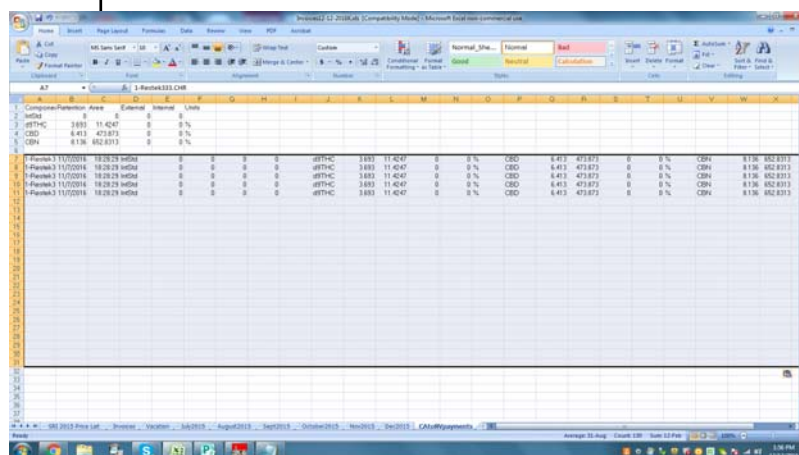
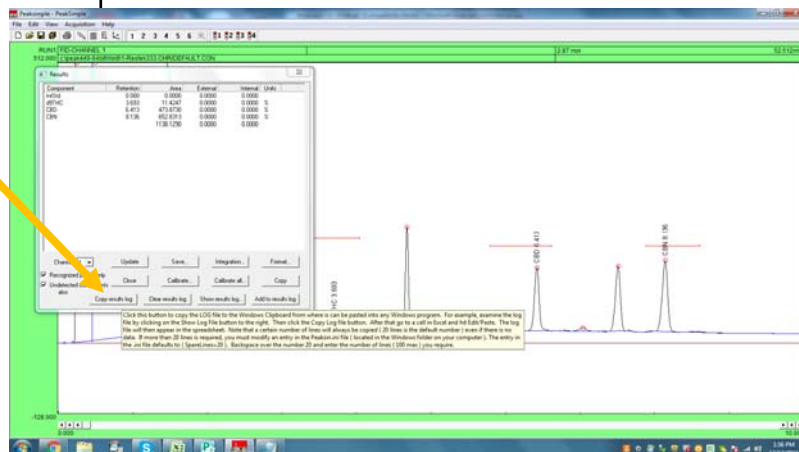
Click the button at the bottom of the Results screen labelled COPY RESULTS LOG.

This copies the entire results log to the Windows clipboard.

In Excel click Paste and the results log loads into Excel.

You can also Load the results log from Excel by clicking File/Open (in Excel) then navigating to the PeakSimple folder to load CH1.log or whatever the name of the log file is.

If the columns of numbers are not perfectly lined up, make sure the box in the results screen labelled UNDETECTED PEAKS ALSO is checked. This reserves a space in the log file for each peak even if it is not detected and has zero area.



Copying Data to Excel December 2016

Page 3

Using the E-mail feature of PeakSimple version 3.84 and later

PeakSimple version 3.84 and later include a e-mail feature which allows the user to send a e-mail containing the results of the chromatogram at the end of every run, or only when an error condition is detected.

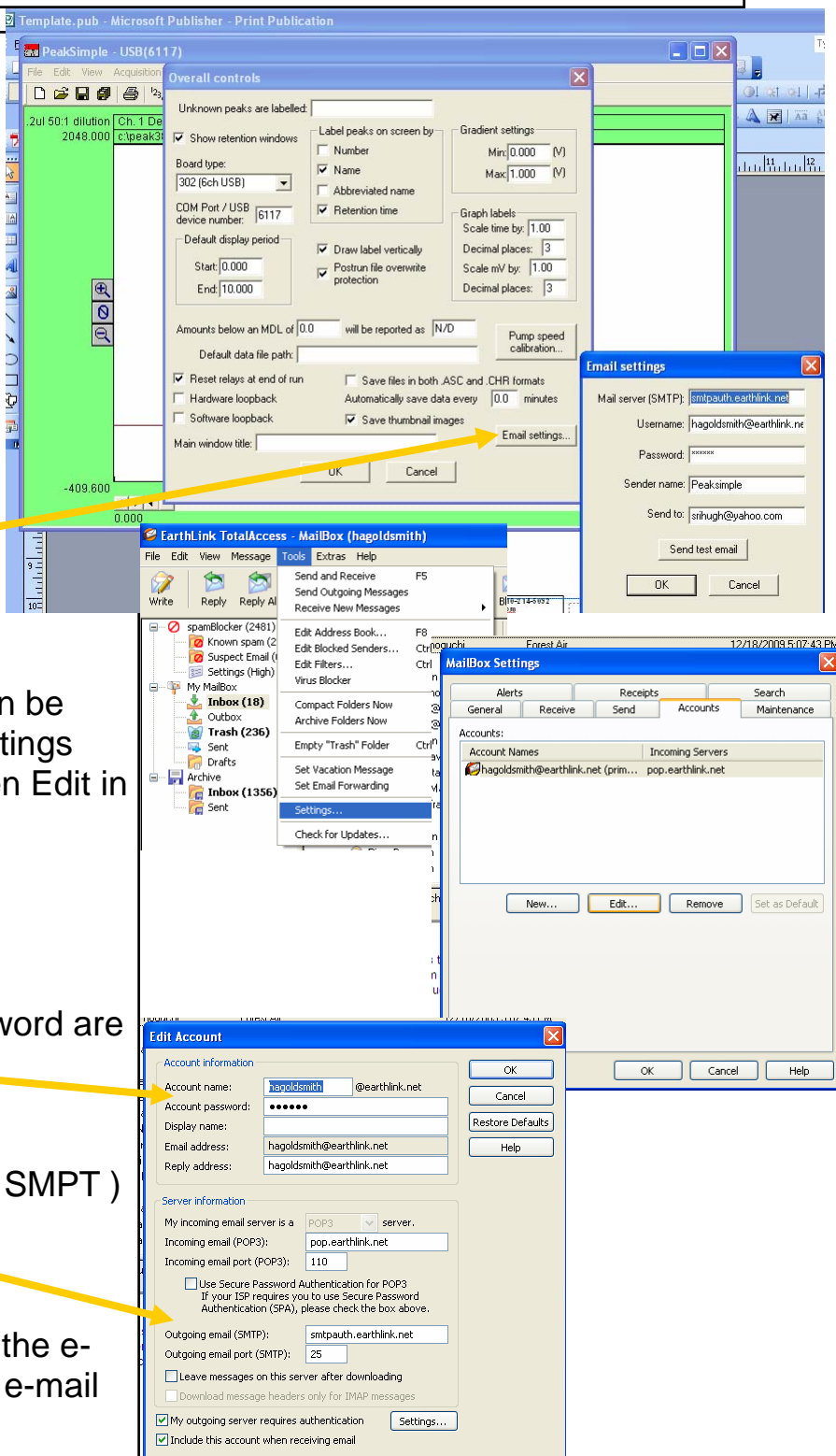
The e-mail send to address is entered in the Edit/Overall screen by clicking the Email Settings button.

Most of this information can be found by clicking Tools/Settings and then Accounts and then Edit in your e-mail application.

The "username" and password are listed here

The outgoing mail server (SMTP) is listed here.

In the "Send To" box enter the e-mail address you want the e-mail sent to.



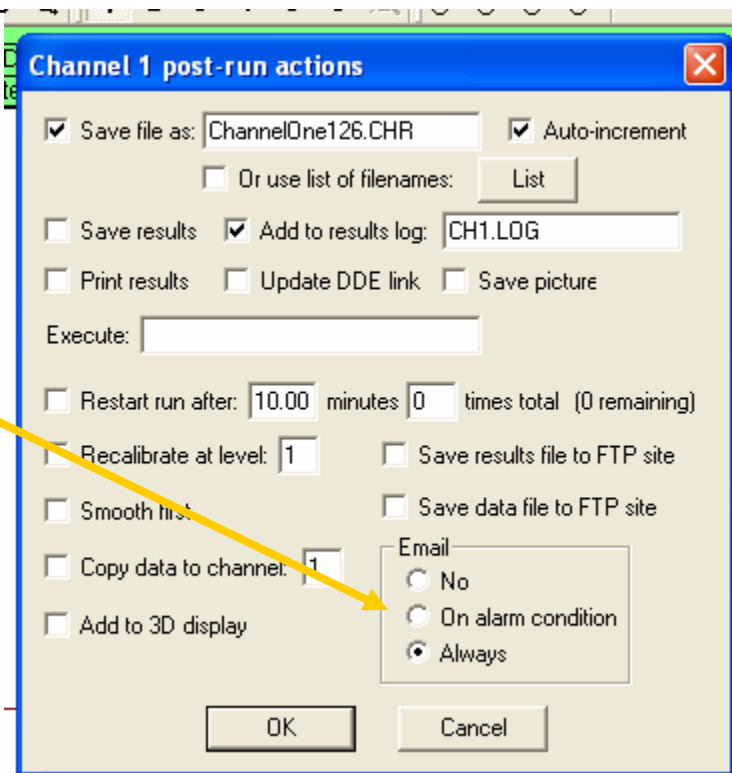
Using the E-mail feature of PeakSimple version 3.84 and later

In the Postrun box for each channel you can select whether to send an e-mail:

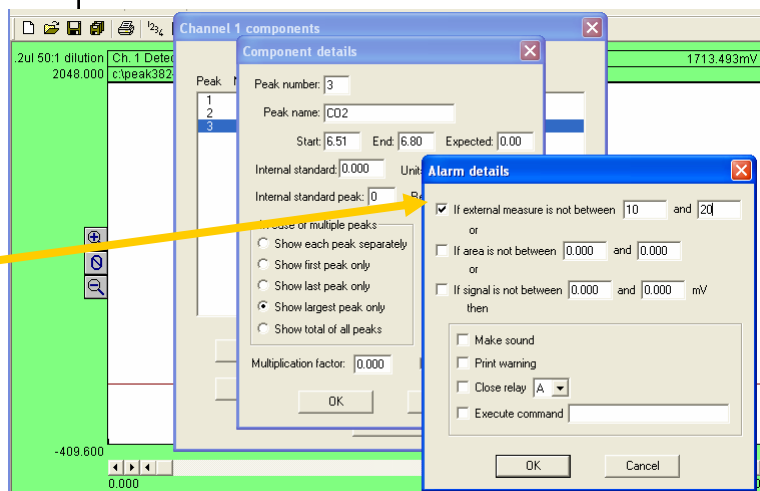
Never (No)

On Alarm Condition only

Always



Set the Alarm conditions in the Components/Details/Alarm Details screen.



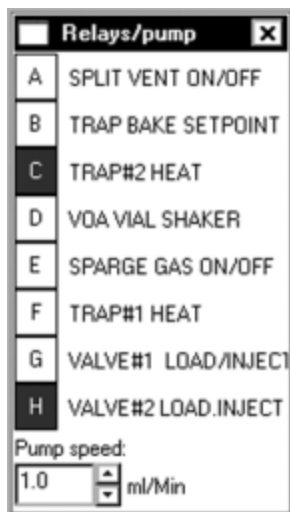
Events

PeakSimple gives you control of up to eight independent external events, or hardware events. A hardware event is the operation of a device external to the data system but integral to the analytical run. A hardware event can be a valve rotation, opening or closing a split vent, activation of an autosampler sequence, or operation of an electrical switch at a precise moment during the run. PeakSimple also gives you control over a comprehensive list of non-hardware events, such as integration events, data system signal control events (zero, reverse), and DOS command events. Events are controlled automatically with **Event tables** that use the system clock, which starts at 0:00 with each run. Using PeakSimple **Event tables** enhances the reproducibility of the resulting chromatograms by ensuring repeatable actuation of devices from run to run.

The eight timed event output signals are called relays, and are named A-H. For example, when an SRI GC is equipped with a 10-port gas sampling valve, its rotation/actuation is controlled by a relay: relay OFF = valve in the LOAD position; relay ON = valve in the INJECT position. The relay assignments for any given instrument are printed on the side panel (right hand side for GCs, left-hand side for HPLCs).

RELAY FUNCTIONS		
(DEFAULT / ACTIVE)		
A	SAMPLE SOLENOID #1	(CLOSED / OPEN)
B	SAMPLE SOLENOID #2	(CLOSED / OPEN)
C	SAMPLE SOLENOID #3	(CLOSED / OPEN)
D	SAMPLE SOLENOID #4	(CLOSED / OPEN)
E	TRAP #1 HEAT	(OFF / ON)
F	TRAP #2 HEAT	(OFF / ON)
G	VACUUM PUMP	(OFF / ON)
H	VALVE #1 POSITION	(LOAD / INJECT)

This list of assigned relay functions is printed on the side of a TO-14 GC customized with 4 sample solenoid valves.

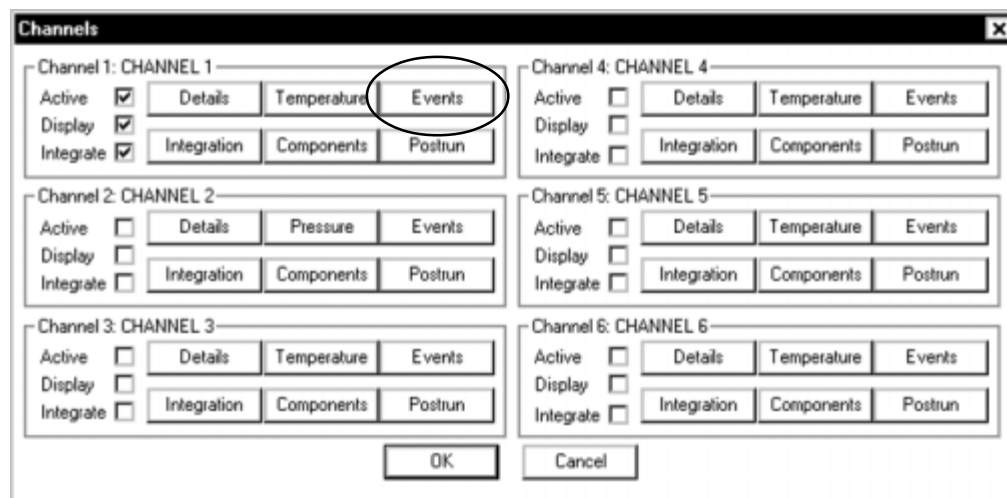


Users may manually control any relay event, either during the run or while in stand-by mode, by using the **Relays/pump** window. Click on View and choose **Relay/pump window**. In this window are eight buttons representing the relays with the appropriate letter. Activate a relay by clicking on its letter; it becomes highlighted to show its ON status. You can also toggle the relays from the keyboard by holding the control key (Ctrl) while pressing the letter of the relay: Ctrl+C, Ctrl+H, etc.

PEAKSIMPLE SOFTWARE

Events

Event Tables



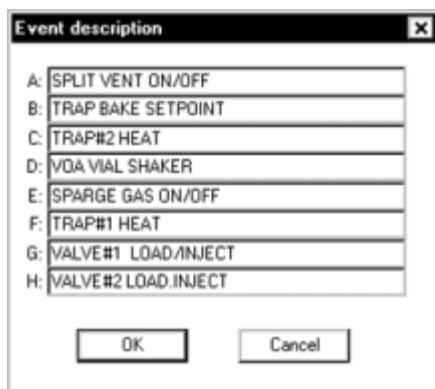
You can open the events table window from the Edit> Channels screen. Click on the Events button for channel 1. Or, right-click in the chromatogram window and select Events from the pop-up menu.



The event table window will open, either empty, or with whatever .EVT file was saved with the current control file (DEFAULT.CON, unless you have specifically opened another). At the bottom of the events table window there are several buttons for you to access event features.

Each channel has its own event table because of the signal processing type events that are available, such as Zero, Reverse, and Integration events. Hardware events may also be activated from any channel. SRI recommends entering hardware events only in the channel 1 event table to avoid confusion.

Click on the **Add...** button to add an event to the event table. The **Event details** screen will open, where you select the event and enter the time at which you want it to occur.



Type in your custom event descriptions.

Click on an existing event in the event table to select and highlight it, then click on the **Change...** button to edit the selected event. You can also simply double-click an event to open the **Event details** screen, from which you can edit any selected event.

Click on the **Remove** button to delete a selected event from the events table.

Click on the **Describe...** button to customize any or all of your eight relay (hardware) event descriptions.

PEAKSIMPLE SOFTWARE

Events

Click the **Load...** button to open an existing event table. PeakSimple will open the program directory and display all .EVT files.

Click **Save...** to save the current event table shown in the window.

Click **Clear** to remove any and all events and .EVT files from the event table window (but not from the hard drive). PeakSimple will prompt you for confirmation before proceeding to clear the event table.

Click the **Print** button to send the current event table to the printer through the Windows print manager.

Channel 1 events

5035-1C.EVT

Time	Event
0.000	ZERO
0.100	E ON (SPARGE GAS ON/OFF)
0.200	D ON (VDA VIAL SHAKER)
5.000	D OFF (VDA VIAL SHAKER)
5.100	E OFF (SPARGE GAS ON/OFF)
6.000	C ON (TRAP#2 HEAT)
6.100	F ON (TRAP#1 HEAT)
8.000	G ON (VALVE#1 LOAD/INJECT)
12.000	E ON (SPARGE GAS ON/OFF)
12.900	E OFF (SPARGE GAS ON/OFF)
13.000	G OFF (VALVE#1 LOAD/INJECT)
13.100	C OFF (TRAP#2 HEAT)
13.200	F OFF (TRAP#1 HEAT)

Click the **Shift...** button to shift the sequence of events following the selected event forward or backward in time.

Shift events

Shift this event and all subsequent events by: 2.000 minutes

OK Cancel

In this example, we are shifting the highlighted event forward 2 minutes.

Channel 1 events

5035-1C.EVT

Time	Event
0.000	ZERO
0.100	E ON (SPARGE GAS ON/OFF)
0.200	D ON (VDA VIAL SHAKER)
7.000	D OFF (VDA VIAL SHAKER)
7.100	E OFF (SPARGE GAS ON/OFF)
8.000	C ON (TRAP#2 HEAT)
8.100	F ON (TRAP#1 HEAT)
10.000	G ON (VALVE#1 LOAD/INJECT)
14.000	E ON (SPARGE GAS ON/OFF)
14.900	E OFF (SPARGE GAS ON/OFF)
15.000	G OFF (VALVE#1 LOAD/INJECT)
15.100	C OFF (TRAP#2 HEAT)
15.200	F OFF (TRAP#1 HEAT)

Add... Change... Remove Describe...

Load... Save... Clear Print

OK Shift...

Now the selected event takes place at 7.00 instead of 5.000; all subsequent events have also been shifted forward two minutes.

The **Shift...** button saves you having to re-type the entire event sequence.

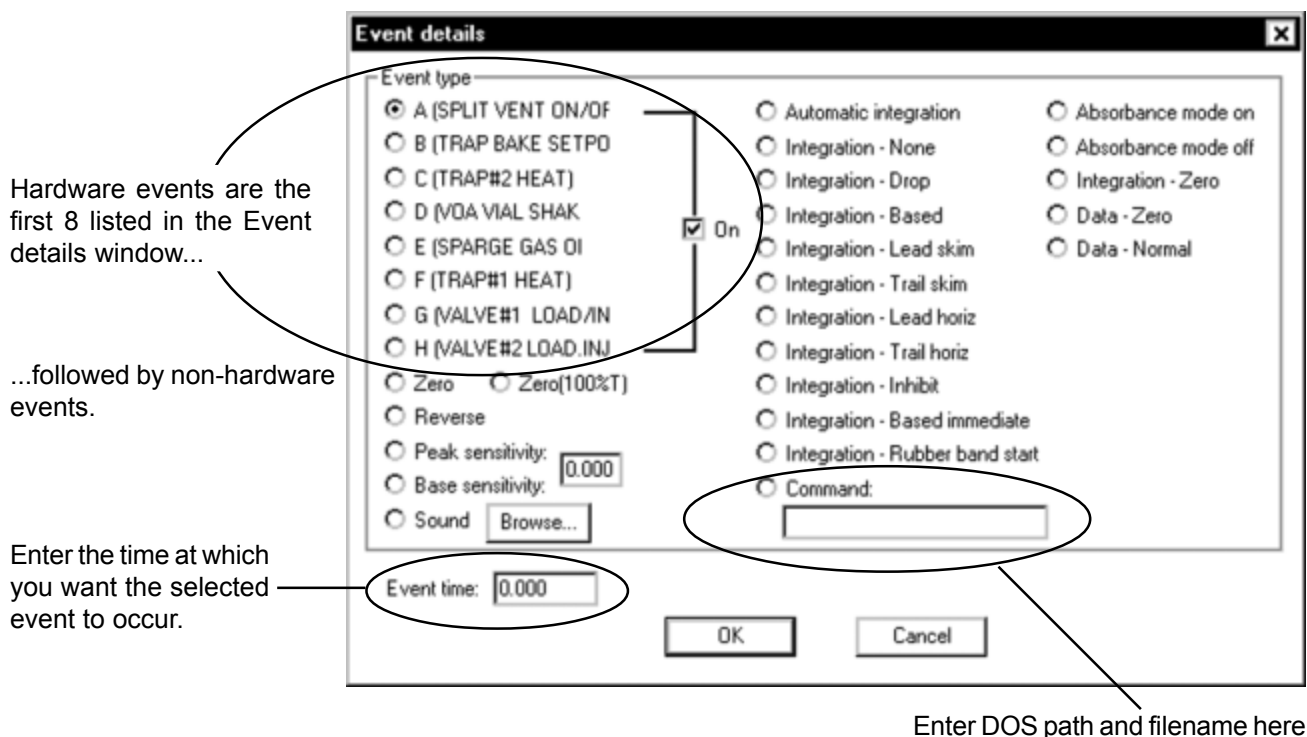
Click the **OK** button to exit the events table window.

PEAKSIMPLE SOFTWARE

Events

The **Event details** screen opens when you click the **Add...** or **Change...** buttons, or when you double-click any single event in the list. In the **Event details** screen are listed all the events you can enter into an event table. Starting on the left, the eight relays are listed, followed by non-hardware events. Hold your mouse cursor over any event to read its ToolTips description.

There is a checkbox labeled “On” to the right of the hardware events list. When the event is turning ON a relay, make sure this box is checked. Uncheck the box when the event is turning OFF a relay. Even though they control the same relay, ON and OFF are separate and distinct events in the timetable. On the bottom left of the Event details window is the Event time field. Enter the time at which you want the event to occur here. Typically, PeakSimple has a lot of tasks to perform at the beginning of an analytical run. Therefore, SRI recommends that you enter the first hardware event no earlier than 0.100 minutes (6 seconds).



PeakSimple also permits you to automatically execute a DOS command during the analytical run using an event table. A DOS command is the same as running an executable file. You may use this function to launch a macro to copy, rename the preceding file so the next file may be updated into a spreadsheet, or to copy the chromatogram data and results file onto a floppy or hard disk drive other than the destination to which it was originally saved. A DOS command may be executed at any time during the analytical run by typing in the DOS path and the filename of an .EXE, .COM, or .BAT file, and the time the event is to occur. To add a DOS command event: click the radio button next to “Command,” and type in your DOS path and executable filename. Example: C:\Excel\Macro1.bat Next, type in the time during the run at which you want the command to be activated in the form field labeled **Event time**. DOS events that require prolonged disk access should be executed after the run, using **Post-run actions** for channel 1.

You can choose to reset all eight relays at the end of the run by clicking Edit>Overall and checking the box in the lower left corner.

This option will return the relays to their default position—OFF.

In some cases, a user may not want to reset the relays at the end of the run. For instance, when using our TO-14 Air Concentrator, users leave the gas sampling valve in the INJECT position at the run's end. This sweeps clean the trap and column, preparing the system for the next sample. In this case, the user would have an event table to turn OFF the valve relay and return it to the LOAD position sometime after the run has started. Therefore, such users would deselect the "Reset relays at end of run" option.

Performing Internal Standard Calibration using PeakSimple version 3.51

For this example, we will create a 5 point calibration curve for Glycerin using Butanetriol as the Internal Standard.

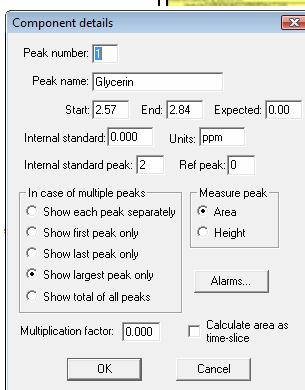
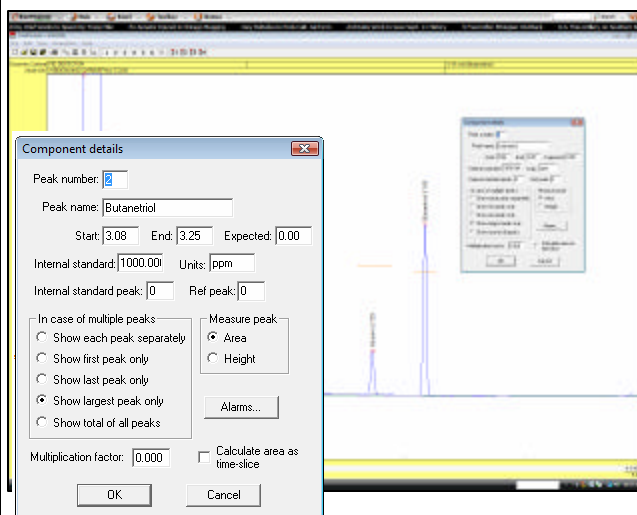
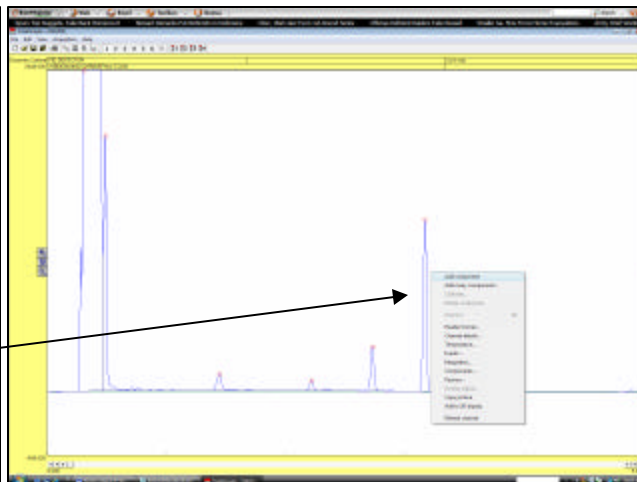
Load the level 1 chromatogram into channel 1. (File/Open)

Identify the Butanetriol Internal Standard peak by using the mouse to point to the Butanetriol peak. Click on the right mouse button, then click Add Component.

Point to the Butanetriol peak again, right click, then select Edit Component (you can just double-click the peak as a short-cut).

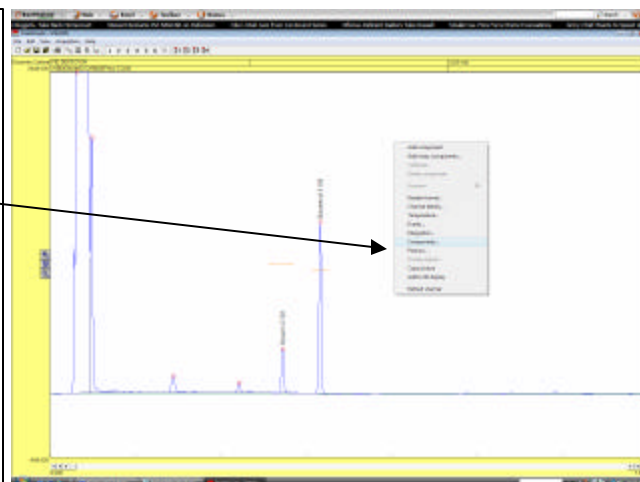
Enter the Component Details especially note that Peak Number is 2 and the Internal Standard is 1000. The Internal Standard is the amount of Butanetriol which you know to be in the sample. In this case it is 1000 ppm.

Go through the same process for Glycerin. Note that the peak number is 1, that the Internal Standard box is left at 0.00, but the Internal Standard Peak box is set to 2. By entering the 2, PeakSimple knows that peak number 2 should be the Internal Standard for this peak (Glycerin).



Performing Internal Standard Calibration using PeakSimple version 3.51

Right click anywhere on the chromatogram screen and select Components



Notice in the Components window that the number 2 is listed in parentheses next to the peak number 1.

Channel 1 components

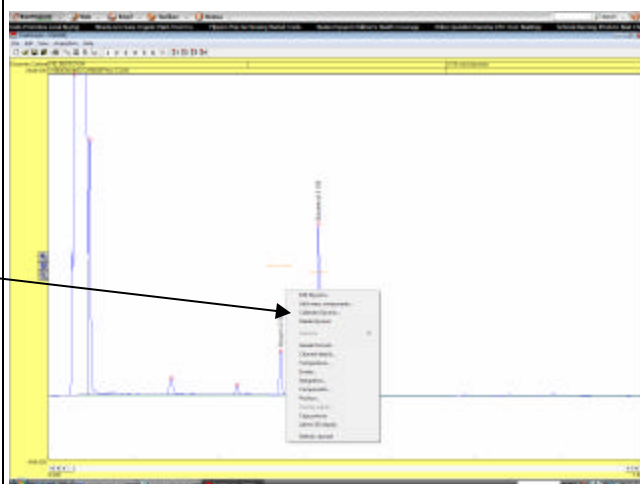
Peak	Name	Start	End	Calibration
1(2)	Glycerin	2.570	2.840	
2*	Butanetriol	3.080	3.250	

Buttons: Add... Change... Remove Calibrate... Load... Save... Clear Print OK

This is how PeakSimple reminds you that peak number 2 (Butanetriol) is the Internal Standard for peak number 1 (Glycerin).

It is a good idea at this point to save the Component table. Click Save and enter a filename (BioDiesel.cpt for example)

Return to the Chromatogram screen, point to the Glycerin peak with your mouse and right click. Select Calibrate Glycerin from the menu.



Performing Internal Standard Calibration using PeakSimple version 3.51

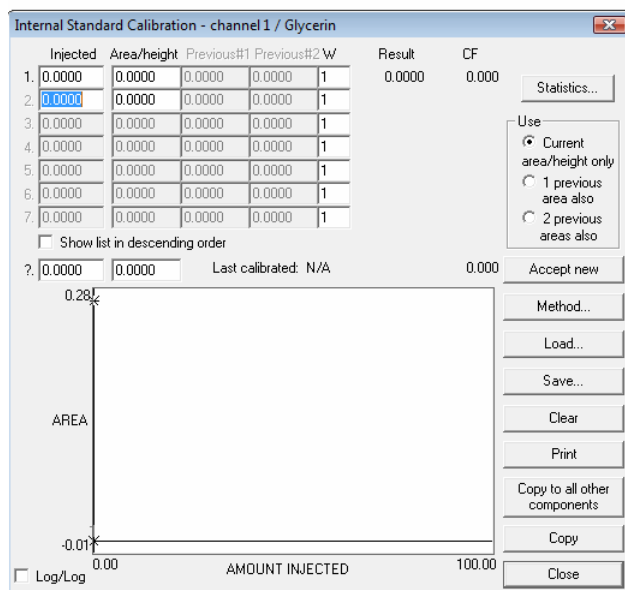
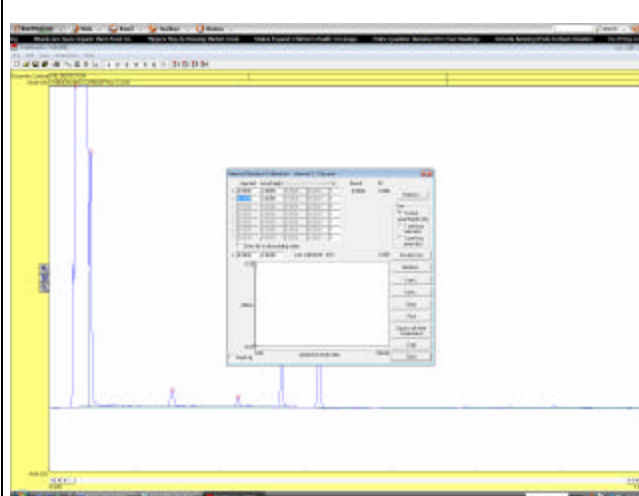
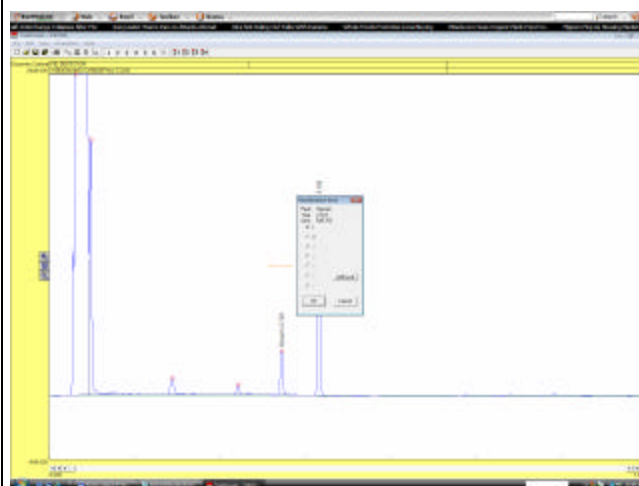
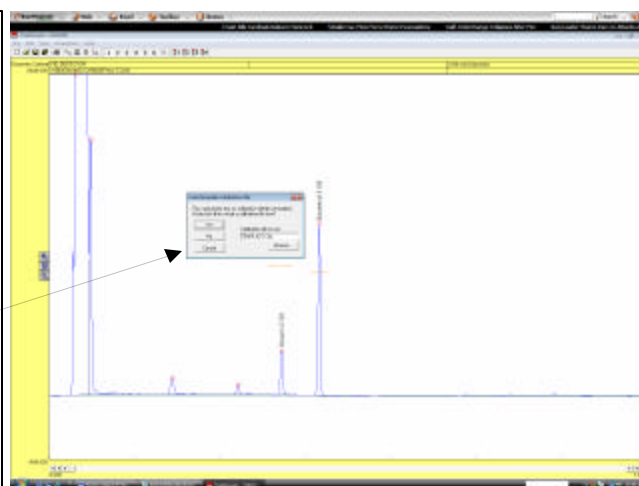
A screen will appear offering to let you copy a Template Calibration file. This is a convenience when creating many calibration curves since you can make a Template calibration curve once and avoid typing in the same information over and over for each similar curve.

We don't need to do this for this example, so just click No.

Another screen appears which allows you to specify the calibration level (i.e. Level 1, Level2, Level 3 etc.).

Since we do not as yet have a curve, click the radio button for Level 1 and then OK.

PeakSimple then displays the blank calibration curve



Performing Internal Standard Calibration using PeakSimple version 3.51

Enter the amount of Glycerin in the Level 1 standard (the chromatogram on the screen). In this example, the Glycerin is at 100ppm, so enter 100 in the top left cell of the table.

Then click on the button labeled Accept New.

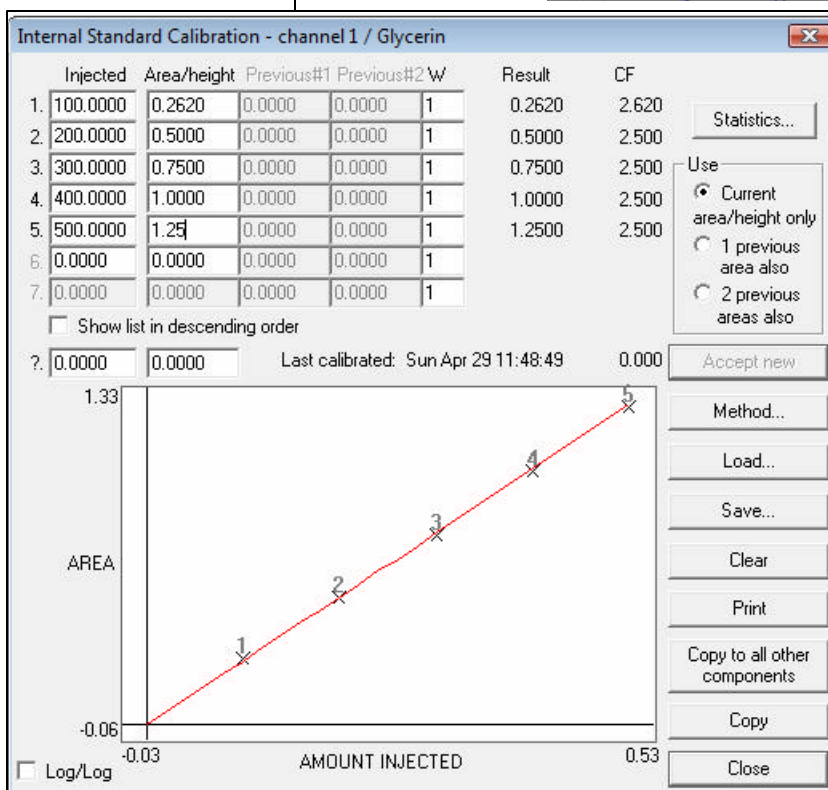
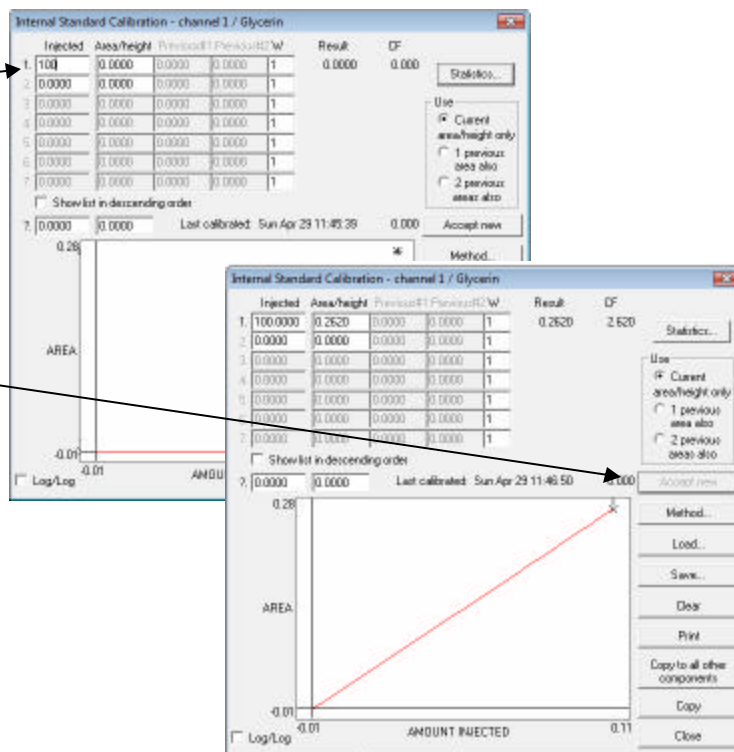
The ratio of the Glycerin peak area divided by the Butanetriol peak area is then entered automatically in the cell immediately to the right of the 100. A single point curve is also drawn on the graph.

It will save time if you enter the remaining Level 2, Level 3 , Level 4 and Level 5 amounts along with estimated ratios.

These are just approximately correct numbers and will be replaced when we actually calibrate Level2 through Level 5.

As you do this you will see the multiple points plotted on the graph.

Save the curve by clicking Save



Performing Internal Standard Calibration using PeakSimple version 3.51

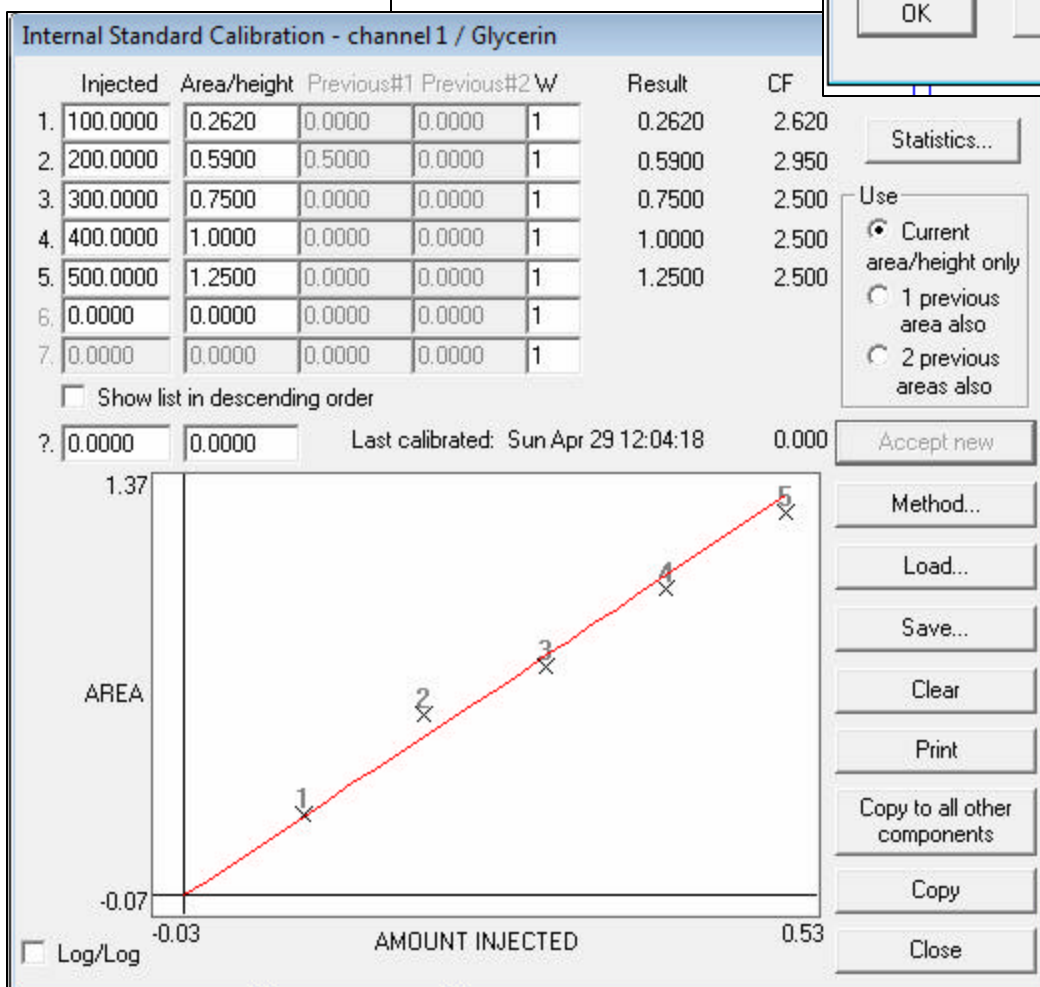
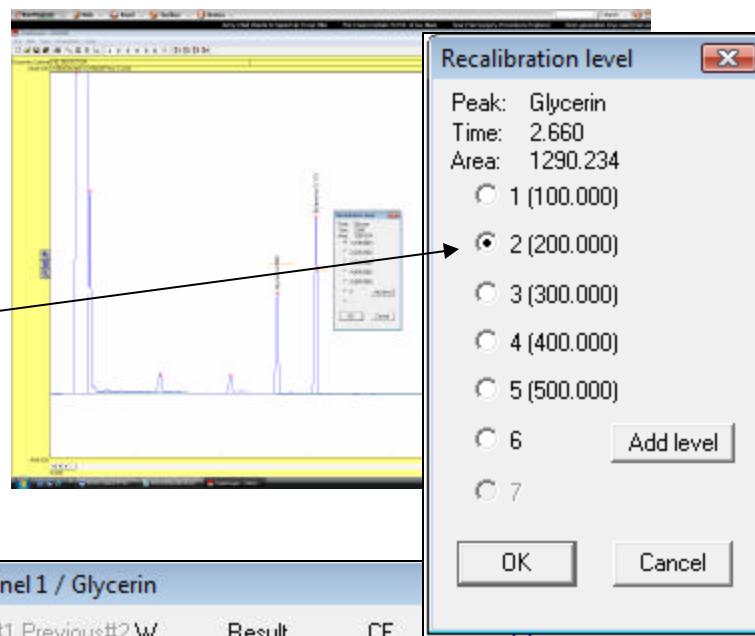
Open the Level 2 chromatogram (File/ Open) or inject the Level 2 standard and allow the run to end. (you can't calibrate until the run is over). Point to the Glycerin peak and right click. From the menu select Calibrate Glycerin.

This time when the Recalibration screen appears, select the Level 2 radio button.

When the Calibration curve screen appears, click Accept New and the ratio between the

Level 2 Glycerin and Butanetriol Internal Standard will be automatically inserted in the Level 2 cell.

Note that the old value (the estimated value we entered previously) is not lost but is shifted one cell to the right.



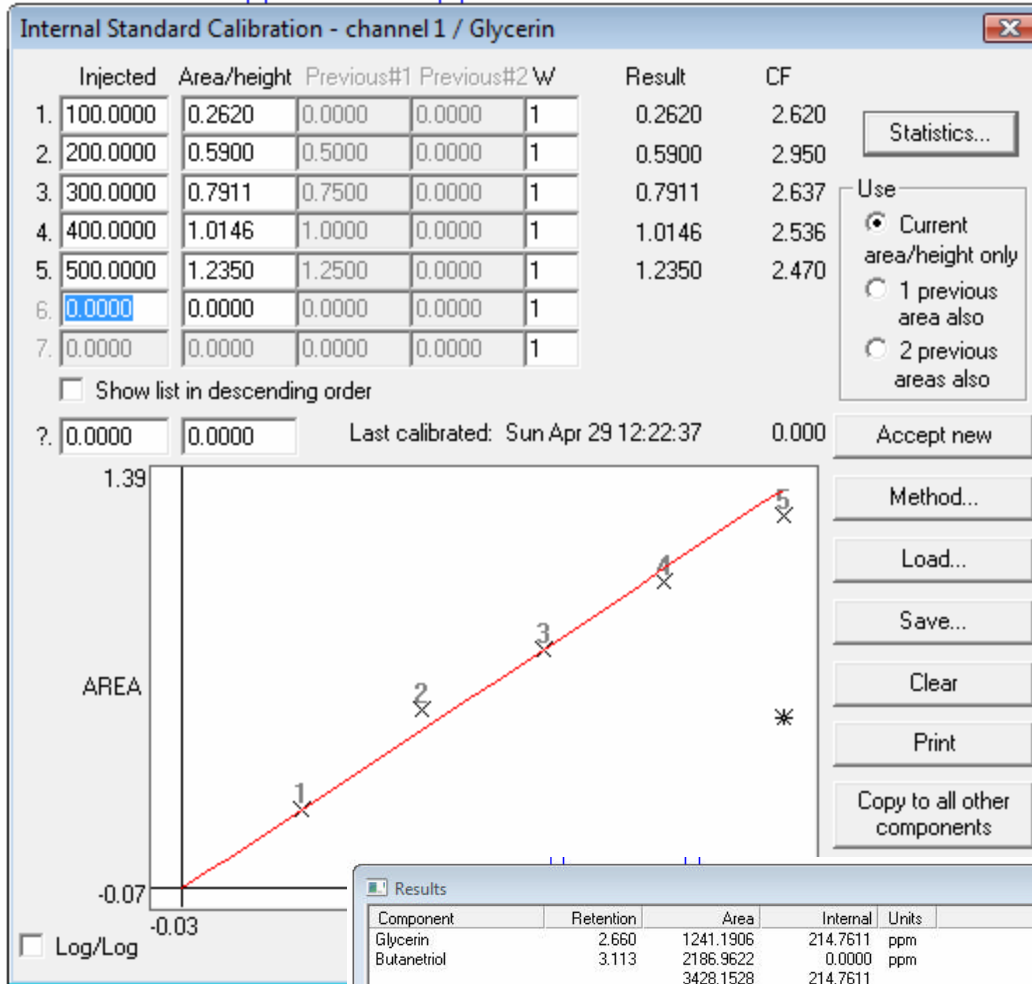
Performing Internal Standard Calibration using PeakSimple version 3.51

Follow the same procedure for Level 3, 4 and 5.

The actual ratios replace the previously entered estimated values to produce a real 5 point calibration curve

Next inject a real sample (not a calibration standard) and verify that the Result screen displays a logical answer under the Internal column.

Note that the Butanetriol Internal Standard peak is not calibrated and shows a 0.00 result.



Results

Component	Retention	Area	Internal	Units
Glycerin	2.660	1241.1906	214.7611	ppm
Butanetriol	3.113	2186.9622	0.0000	ppm
		3428.1528	214.7611	

Channel: 1 Update Save... Integration... Format...

☒ Recognized peaks only ☐ Undetected components also

Close Calibrate... Calibrate all... Copy

Copy results log Clear results log Show results log... Add to results log

Enabling the Pressure program on the SRI 8610C GC

The A/D board is mounted along the inside right side of SRI 8610C, 310C and 410 GCs.



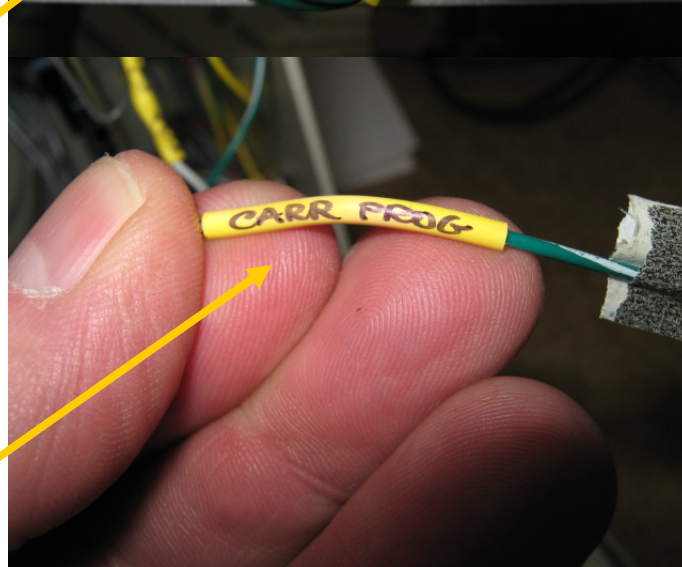
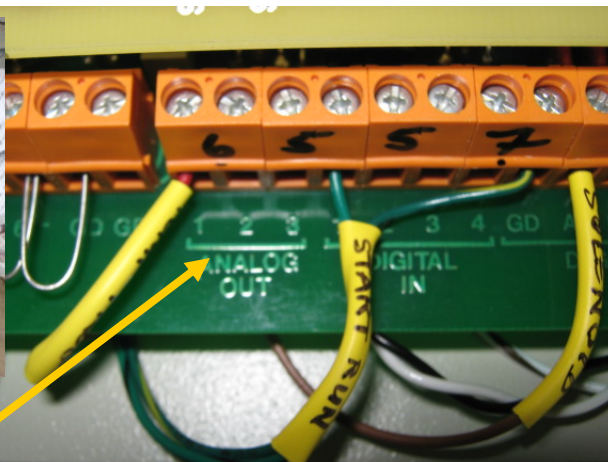
The A/D board is labeled Analog Out 1,2 and 3 if your A/D board is a model 302 6 channel USB type.

The 302 board has 3 analog outputs. Analog output #1 is used to control the oven temperature program. Analog outputs #2 and 3 are normally left unconnected to anything.

All other A/D boards (model 333, model 202 and model 203) are labeled TP1 (temperature program one) or TP2 (temperature program two). These board only have two analog outputs.

Locate the wire which is labeled Carr Prog (carrier program). This wire will be tucked under the A/D board and insulated with a piece of colored tape.

Connect the Carr Prog wire to Analog output #2 (or TP2) to enable the program in PeakSimple's Channel Two to control the carrier gas pressure. If you prefer, you can connect to Analog output #3 in which case the program in PeakSimple's channel 3 would control the carrier gas pressure.



Enabling the Pressure program on the SRI 8610C GC

Set the "Control By" radio button in PeakSimple's Channel Two details screen to "Pressure".

Channel 2 details

Description: **FID-CHANNEL 1** End time: **11.000** min

Sample rate:
☐ 1 Hz
☐ 2 Hz
☒ 5 Hz
☐ 10 Hz
☐ 20 Hz
☐ 50 Hz

Default display limits:
 Max: **2.000** mV
 Min: **-2.000** mV

☒ Remote start
 Timebase:
☒ 1
☐ 2
☐ 3
☐ 4

Control by:
☐ Temperature
☒ Pressure
☐ Gradient

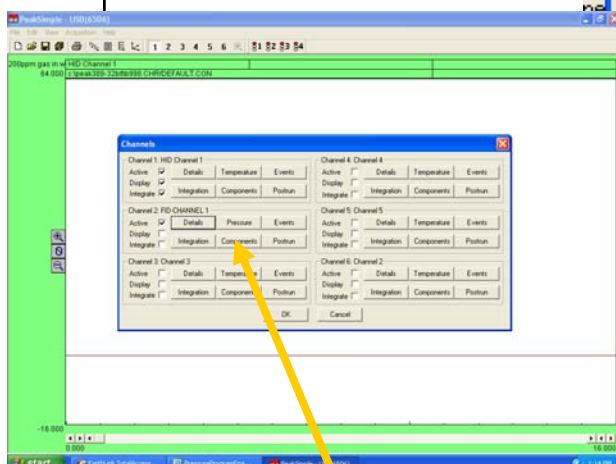
☐ Subtract baseline in channel: **1**
☐ Overlay data in channel: **1**

Relative retention shifts are based at: **0.000** min
 Unretained solute time: **0.000** min

☐ Reverse polarity ☐ Absorbance mode

Multiply norm area % results by: **1.0000**

Datalogger mode:
☐ On
 Offset: **0.000**
 Gain: **1.000**
☐ Use calibration from component:
0
 Decimal places: **-1**



Exit the Channels menu and then re-enter. You will see that the Channel 2 Temperature button is now labeled Pressure

Enter a pressure program which is appropriate for your analysis.

Channel 2 pressure control

C:\peak388-32bit\Vertical.flo

Init PSI	Hold	Ramp	Final PSI
10.00	1.000	1.000	20.00

Graph showing pressure (PSI) vs. time (min). The pressure starts at 10.00 PSI, holds for 1.000 min, then ramps up to 20.00 PSI at 11.000 min.

Buttons: Add... Change... Remove Load... Save... Clear Print OK

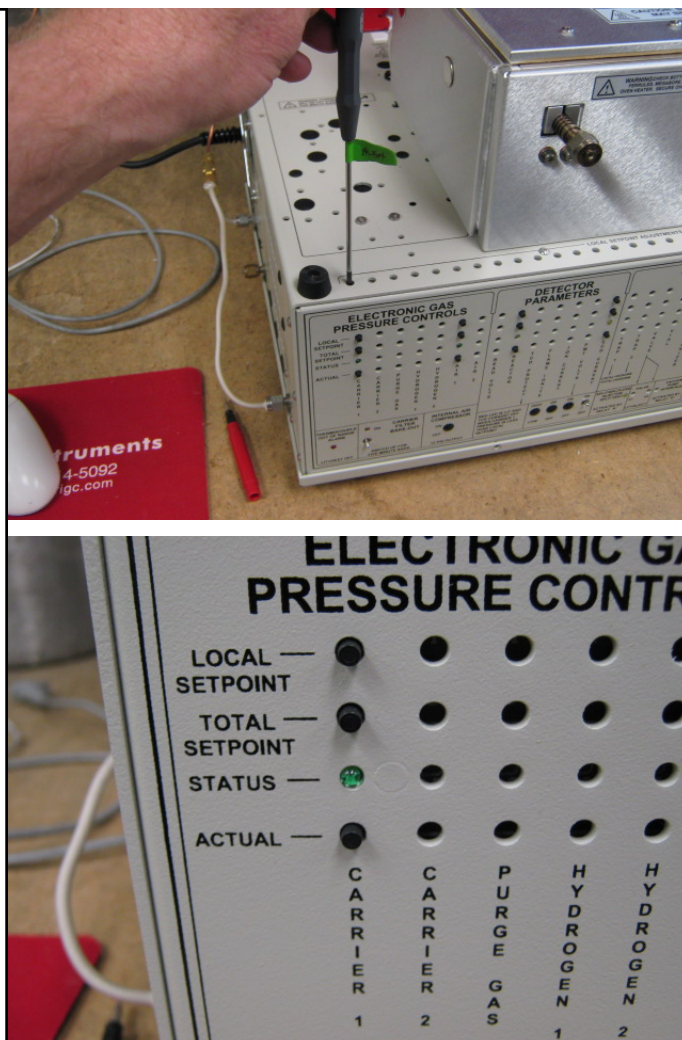
Enabling the Pressure program on the SRI 8610C GC

Using a screwdriver adjust the Carrier Local Setpoint to 000. The Total Setpoint will now display whatever Channel Two pressure program is set to.

The Total Setpoint is the sum of the local setpoint (the screwdriver setpoint) and the remote setpoint (the setpoint from PeakSimple).

If the local setpoint is set to something other than 000 it will add to the Total Setpoint. So if the local setpoint was 5 and the remote setpoint was 5, the Total Setpoint would read 10.

When the GC is first turned on and before PeakSimple establishes communication, or if Channel Two is not activated the remote setpoint defaults to 45psi.



PEAKSIMPLE SOFTWARE

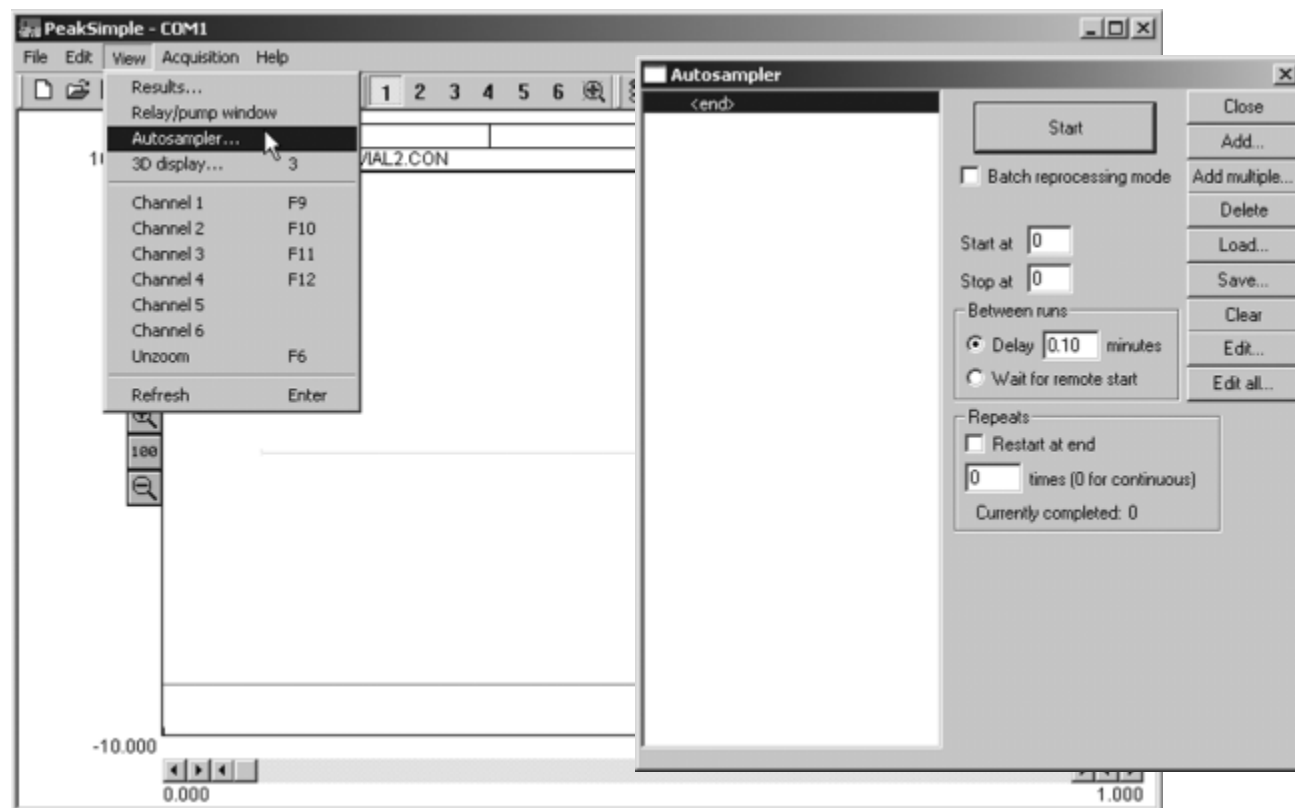
Autosampler Queue

The Autosampler Queue is the most powerful and complex function of PeakSimple, and requires a thorough understanding of the software's features. If you are at the beginner level, you should not attempt to use this feature.

The Autosampler Queue allows a list of control files to be run automatically in sequence. PeakSimple uses control files to save the operating settings of specific methods. Once all the user-definable parameters have been set, they can be saved in a control file for future use. Control files contain .CAL, .CHR, .CPT, .EVT, .GRA, and .TEM files, and every other user-modifiable parameter. You must begin with control files already made, to load into the Autosampler Queue. You must create or modify a control file for each vial.

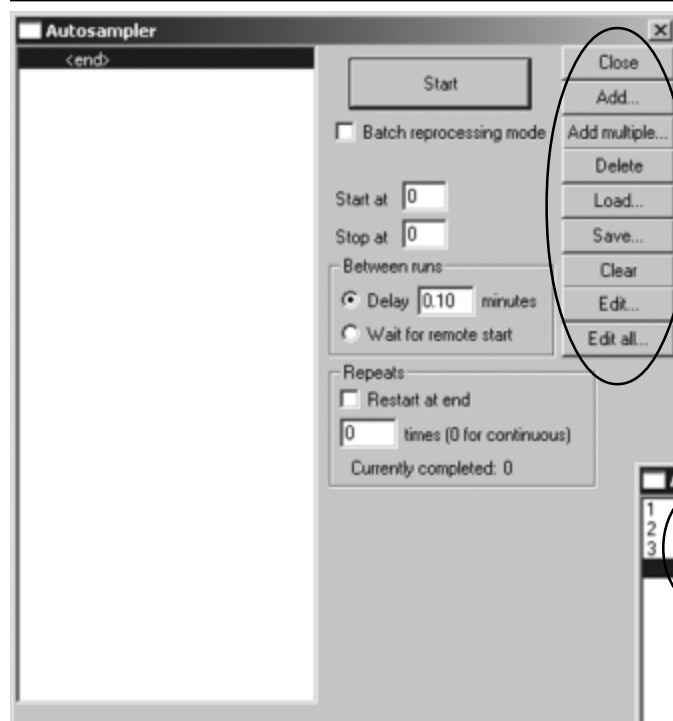
Each control file in the list must have a unique name, even if it is identical to others. It is helpful to include a number in the name of each control file that corresponds with its place in the list; for example: Vial01.con, Vial02.con, Vial03.con, etc. The control file(s) you wish to use in the Autosampler Queue must be saved in the PeakSimple application directory.

To open the Autosampler window, click View, then choose Autosampler.



PEAKSIMPLE SOFTWARE

Autosampler Queue

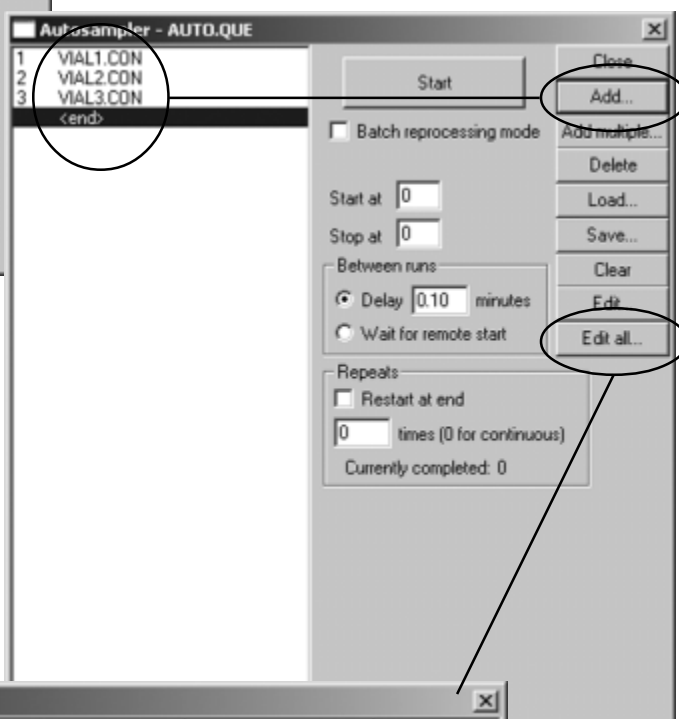


Autosampler Queue Buttons

There are several buttons on the right-hand side of the autosampler window. The **“Close” button** is for closing the Autosampler window. The **“Add” button** is for adding control files to the queue. Click the “Add...” button. Browse to the PeakSimple application directory, and select a control (.CON) file to place in the queue. PeakSimple will place the file in the queue above the .CON file you have highlighted, or at the end of the list if “<end>” is highlighted (default).

Since you can only add one control file to the queue at a time, it can get tedious, especially if you are using multiple instances of the same control file.

When this is the case, use the “Add...” button to add your master control file to the queue, then click on the “Edit all” button to open the control file attributes spreadsheet, shown below.



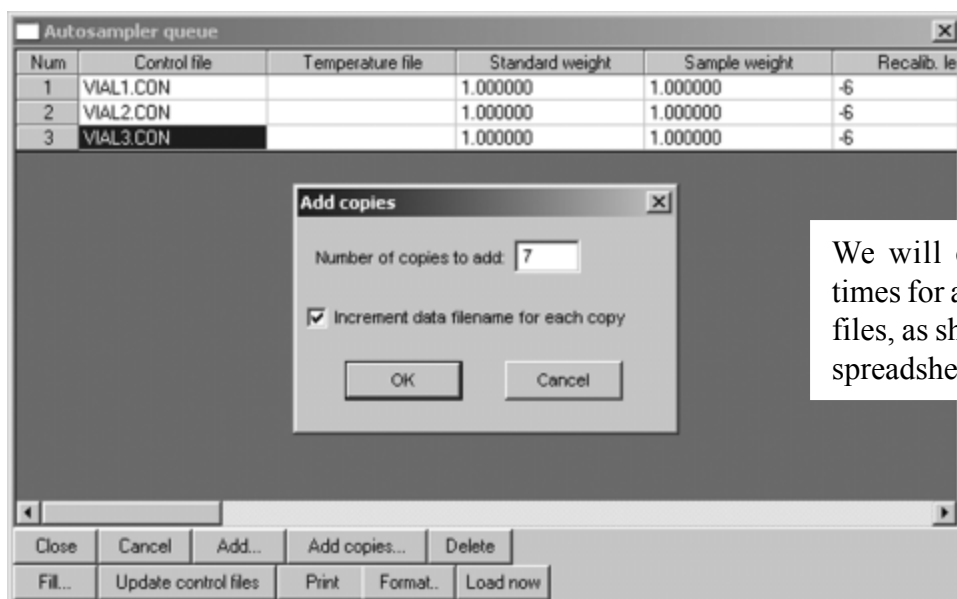
Autosampler queue					
Num	Control file	Temperature file	Standard weight	Sample weight	Recalib. le
1	VIAL1.CON		1.000000	1.000000	-2
2	VIAL2.CON		1.000000	1.000000	-2
3	VIAL3.CON		1.000000	1.000000	-2

PEAKSIMPLE SOFTWARE

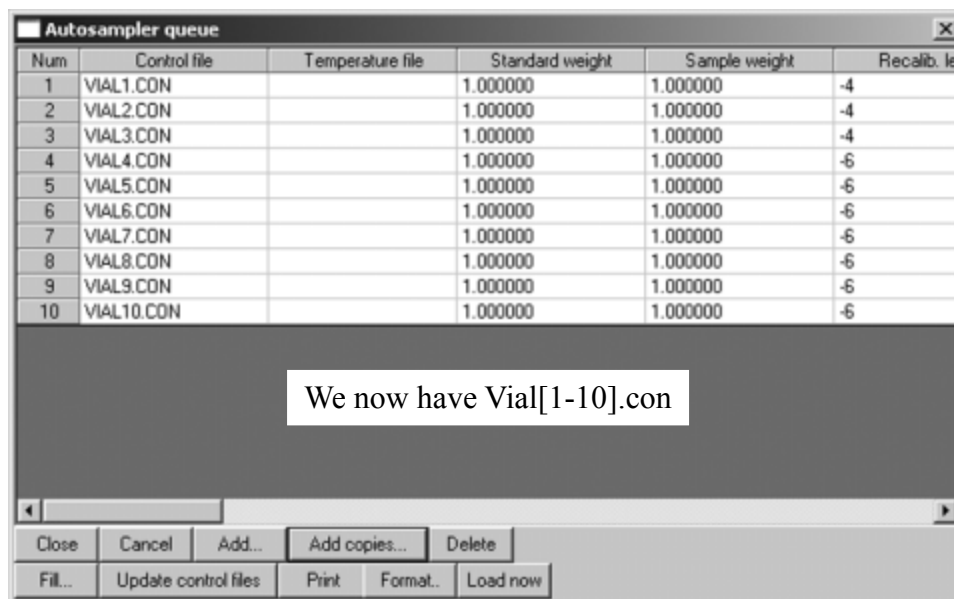
Autosampler Queue

Highlight the control file that is your master, or the one that is to be repeated, and click the “Add copies” button. In the window that pops up, enter the number of copies you wish to make, and check the “Increment data filename for each copy” box. PeakSimple will save the copied control files in the application directory.

The following example is for a 10 vial liquid autosampler for GC. In this example, we have three control files. The third control file is the one we will copy.



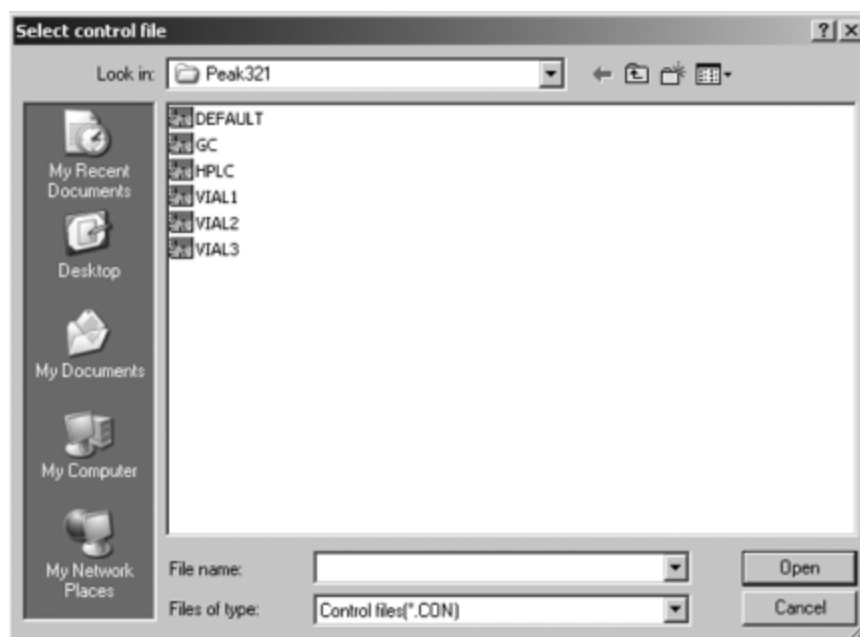
We will copy Vial3.con 7 times for a total of 10 control files, as shown in the Edit all spreadsheet below.



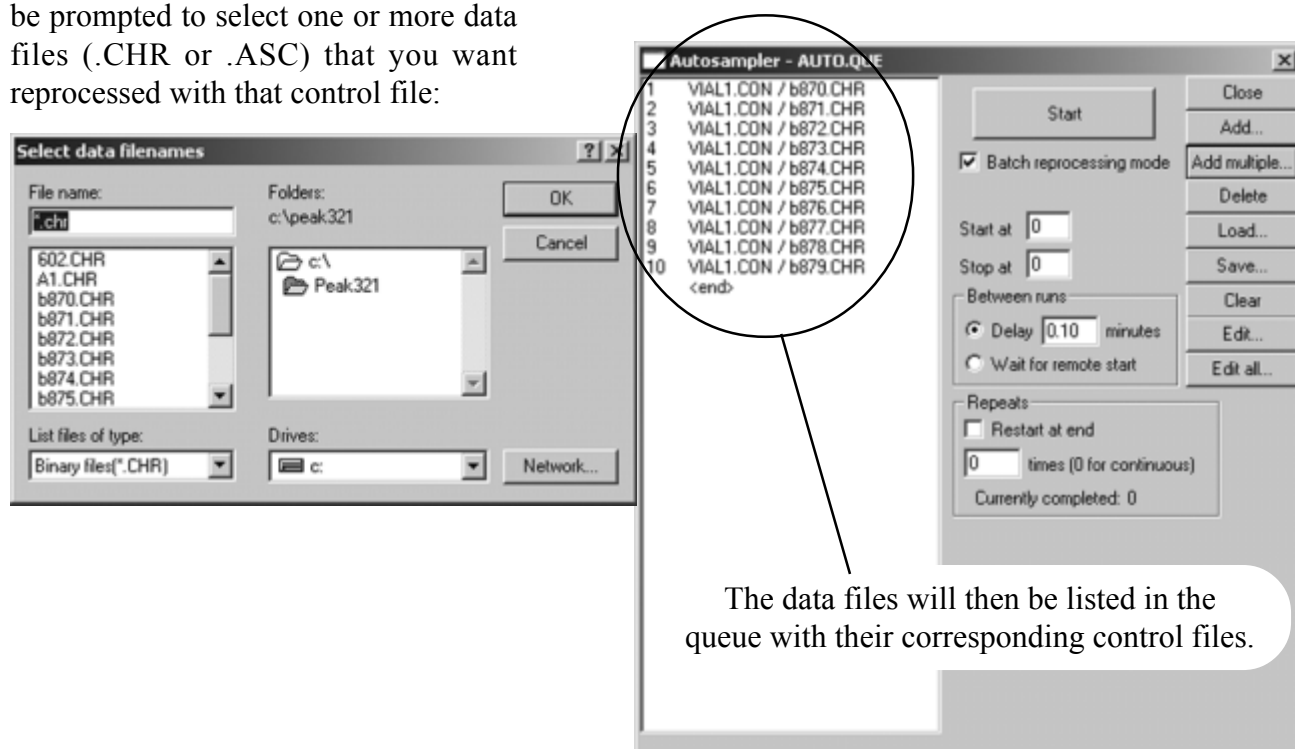
PEAKSIMPLE SOFTWARE

Autosampler Queue

The “**Add multiple**” button is for batch reprocessing. Batch reprocessing allows you to reprocess the raw data through a designated control file. This is useful in the event of a mistake or omission, or when header/comment info needs updating. The “Batch reprocessing mode” checkbox to the left of the “Add multiple” button must be selected. Then, when you click the “Add multiple” button, you will be prompted to select a control file:

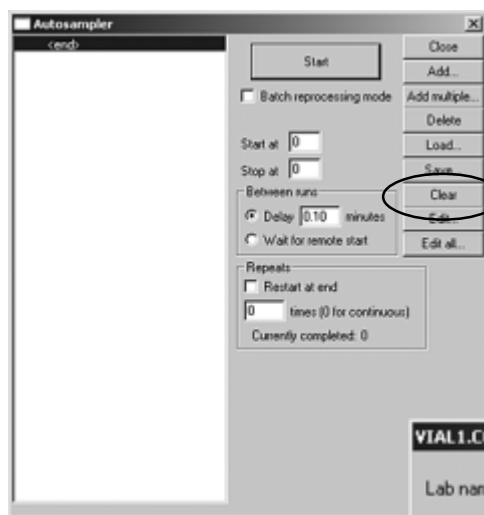
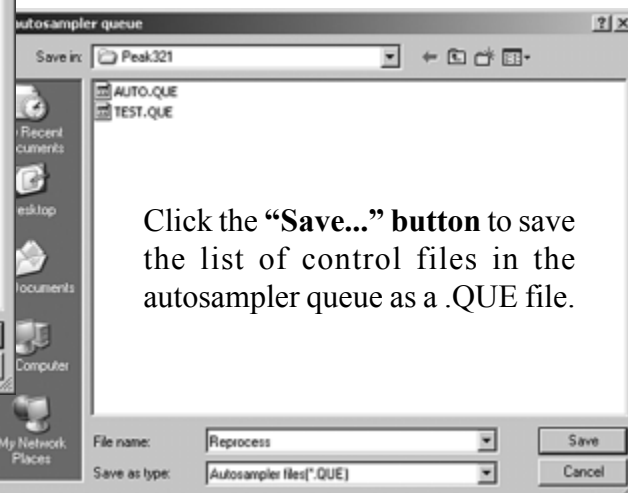
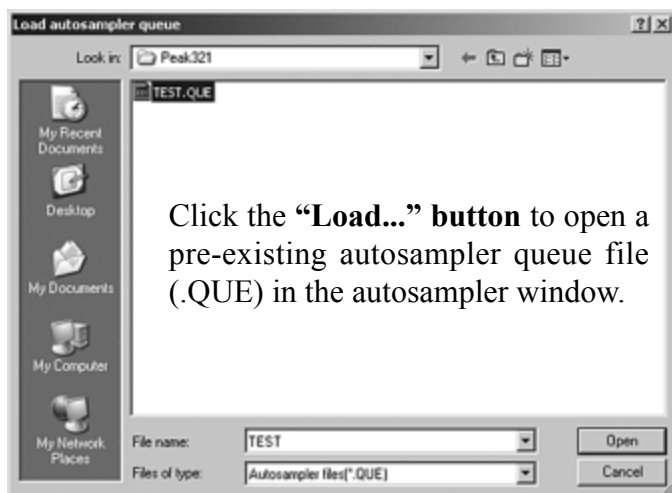


When you select a control file, you will be prompted to select one or more data files (.CHR or .ASC) that you want reprocessed with that control file:



PEAKSIMPLE SOFTWARE Autosampler Queue

To delete a control file from the autosampler queue, highlight it and click the **“Delete”** button. If no control file is highlighted, the last file in the list will be deleted when this button is clicked.



When you click the **“Edit...”** button after highlighting a control file in the queue, the control file is loaded and a screen opens in which you can edit common parameters. To edit other parameters of the control file, just close the “Edit” screen, then click on the PeakSimple window behind the Autosampler window to make the changes. Click File>Save control file when you are finished editing.

Lab name	SRI RUN#1	Data file	C:\Peak321\vb874.CHR
Client		Component file	QUEUE.CPT
Client ID		Event file	
Collection date		Temperature I	
Holding time		Sample	VIAL1
Method		Operator	
Lab ID		QC batch number	
Description	1ST AUTOSAMP RUN	Standard weight	1.000
Column	RESTEK 15METER MXT-1	Sample weight	1.000
Carrier	HELIUM AT 300 ON DIAL	Recalibration level	0
		Add to results log	<input type="checkbox"/>

Channel: 1 (selected), 2, 3, 4, 5, 6

OK Cancel

PEAKSIMPLE SOFTWARE

Autosampler Queue

Click on the **“Edit all...”** button to open the control file attributes spreadsheet. The Edit all spreadsheet is a powerful tool for managing your control files; it allows you to edit any or all of the control files in the autosampler queue.

You can highlight an entire column to change...

...Or make changes in individual cells.

Autosampler queue

Num	Control file	Lab name	Client	Client ID	Collectio
84	Sample80.CON	SRI RUN#2			
85	Sample81.CON	SRI RUN#2			
86	Sample82.CON	SRI RUN#2			
87	Sample83.CON	SRI RUN#2			
88	Sample84.CON	SRI RUN#2			
89	Sample85.CON	SRI RUN#2			
90	Sample86.CON	SRI RUN#2			
91	Sample87.CON	SRI RUN#2			
92	Sample88.CON	SRI RUN#2			
93	Sample89.CON	SRI RUN#2			
94	Sample90.CON	SRI RUN#2			
95	Sample91.CON	SRI RUN#2			
96	Sample92.CON	SRI RUN#2			
97	Sample93.CON	SRI RUN#2			
98	Sample94.CON	SRI RUN#2			
99	Sample95.CON	SRI RUN#2			

Autosampler queue

Num	QC batch	Standard weight	Sample weight	Lab name(2)	Clier
84		1.000000	1.000000	SRI Instruments	
85		1.000000	1.000000	SRI Instruments	
86		1.000000	1.000000	SRI Instruments	
87		1.000000	1.000000	SRI Instruments	
88		1.000000	1.000000	SRI Instruments	
89		1.000000	1.000000	SRI Instruments	
90		2.000000	1.000000	SRI Instruments	
91		1.000000	1.000000	SRI Instruments	
92		1.000000	1.000000	SRI Instruments	
93		1.000000	1.000000	SRI Instruments	
94		1.000000	1.000000	SRI Instruments	
95		1.000000	1.000000	SRI Instruments	
96		1.000000	1.000000	SRI Instruments	
97		1.000000	1.000000	SRI Instruments	
98		1.000000	1.000000	SRI Instruments	
99		1.000000	1.000000	SRI Instruments	
100		1.000000	1.000000	SRI Instruments	

Buttons: Close, Cancel, Add..., Add copies..., Delete, Fill..., Update control files, Print, Format..., Load now

There are ten buttons on the lower left corner of the “Edit all” spreadsheet.

Click on the **“Close”** button to close the spreadsheet window with a prompt to save your changes.

To close the spreadsheet window without saving any changes, click the **“Cancel”** button.

Click the **“Add...”** button to add a control file to the queue and spreadsheet.

Use the **“Add copies...”** button to add copies of a selected control file to the queue.

Click the **“Delete”** button to remove a highlighted control file from the queue. If no control file is highlighted, the last file in the list will be deleted when this button is clicked.

PEAKSIMPLE SOFTWARE

Autosampler Queue

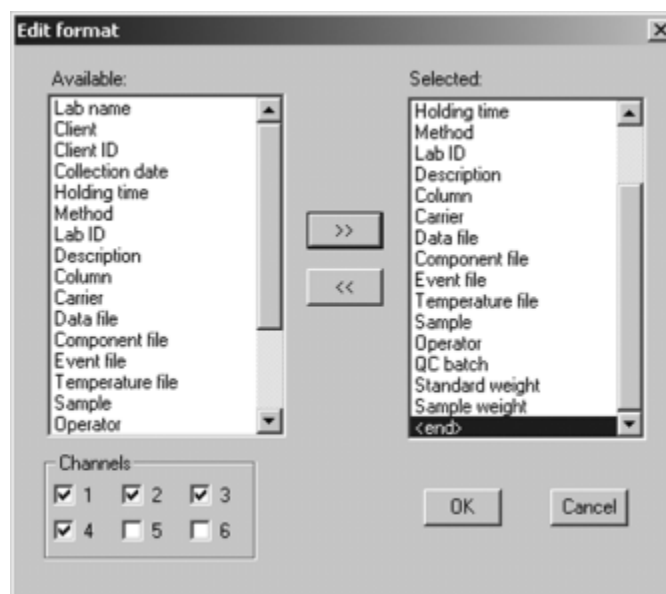
Use the **“Fill...”** button after highlighting a vertical column in the spreadsheet to fill the cells with new text. To highlight a vertical column, click in the uppermost cell you want to include, then drag your cursor down to the last cell you want included.

Num	Control file	Lab name	Client	Client ID	Collectio
84	Sample80.CON	SRI RUN#2			
85	Sample81.CON	SRI RUN#2			
86	Sample82.CON	SRI RUN#2			
87	Sample83.CON	SRI RUN#2			
88	Sample84.CON	SRI RUN#2			
89	Sample85.CON	SRI RUN#2			
90	Sample86.CON	SRI RUN#2			
91	Sample87.CON	SRI RUN#2			
92	Sample88.CON	SRI RUN#2			
93	Sample89.CON	SRI RUN#2			
94	Sample90.CON	SRI RUN#2			
95	Sample91.CON	SRI RUN#2			
96	Sample92.CON	SRI RUN#2			
97	Sample93.CON	SRI RUN#2			
98	Sample94.CON	SRI RUN#2			
99	Sample95.CON	SRI RUN#2			
100	Sample96.CON	SRI RUN#2			

Buttons: Close, Cancel, Add..., Add copies..., Delete, Fill..., Update control files, Print, Format..., Load now

Click the **“Update control files”** button to save all the changes made to the control files in the spreadsheet.

Click the **“Format...”** button to specify which control file parameters are displayed in the spreadsheet. Some commonly edited control file parameters are included by default, but the user may format the “Edit all” spreadsheet as desired. For example, if you have one detector, you can format the spreadsheet to display the parameters for one channel instead of all six (regardless of your GC and data system specs, PeakSimple always has six channel capability). To add a column to the spreadsheet, highlight the header in the list on the left, then click the double right arrow (>>). The header will appear in the list on the right, which is the list of selected features/column headers. To remove a header and column from the spreadsheet, highlight it in the “Selected” list, then click the double left arrow (<<).



Highlight a control file and click the **“Load now”** button to open it in the main PeakSimple window for editing.

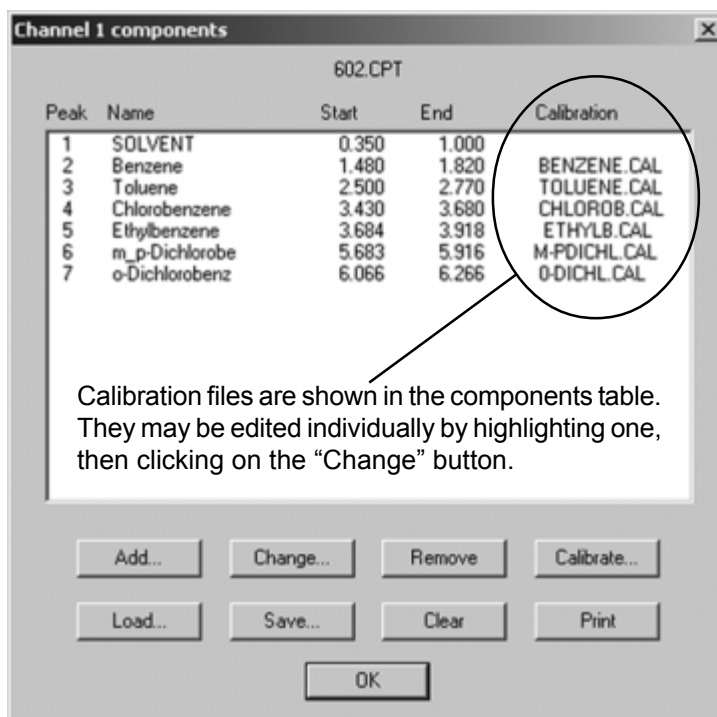
PEAKSIMPLE SOFTWARE

Autosampler Queue

Calibration

The calibration curve is calculated from user-generated results obtained at several different concentrations that span the expected range to be encountered in actual samples. Calibration is required for each component you expect to be in your sample, and for each detector you will be using in your analysis. Once calibration curves have been completed and calibration files saved, they will be included in the .CPT file.

It is typical to calibrate samples at the beginning of an autosampler queue. Remember, the calibration curve is calculated from user-generated results obtained at several different concentrations that span the expected range to be encountered in actual samples. You must have already created your calibration curves before using the Autosampler queue.



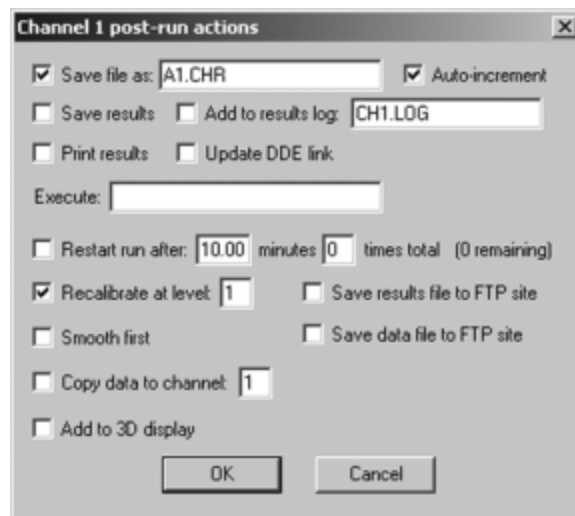
To make the first 3 vials calibration standards:

1. In PeakSimple, click "File," then choose "Open control file." Browse to the application directory, where you should already have saved the control files you want to use in the Autosampler queue. Select the control file that you want to run first. For each channel, open the post-run actions window, and select the "Recalibrate at level" box. Enter "1" in the box. Click "File" then choose "Save control file."

2. Open the second control file in the Autosampler queue and do the same for each channel, except enter a "2" in the box. Save the second control file.

3. Repeat the steps for the third control file, except enter a "3" in the box. You can also edit the control files through the "Edit all" spreadsheet in the Autosampler queue.

In the post-run actions window, the "Recalibrate at level ____" check box recalibrates all identified peaks at the end of a run. The level of recalibration, from 1 to 7, is typed in by the user.

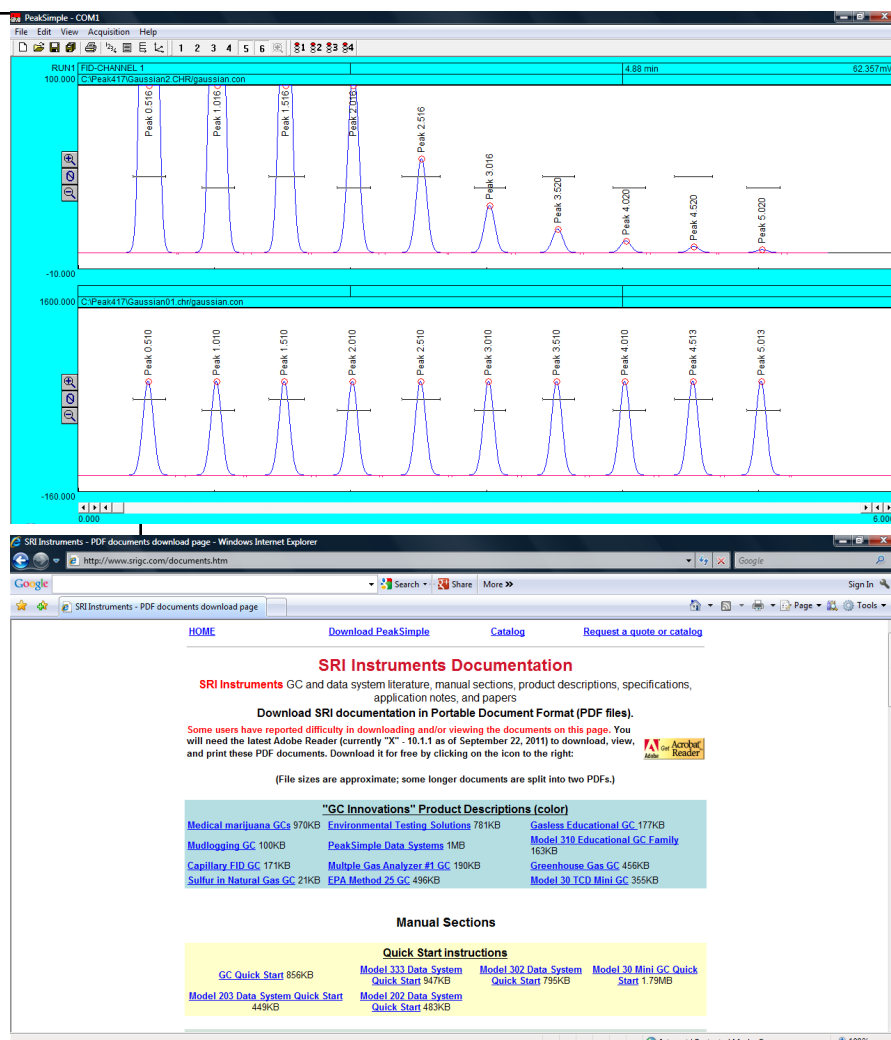


PeakSimple Software Self Validation

PeakSimple is SRI's software that allows a GC to communicate and interface with a Windows computer through an A/D (analog to digital) converter. The latest version can be downloaded for free from www.srigc.com.

Download the validation data package from www.srigc.com. Place the three files (Validation components.cpt, Reproducibility.chr, and Linearity.chr) into a folder on your C: drive named "Validation" (C:\Validation).

In order to validate the PeakSimple software the user will employ either **Hardware loopback** or **Software loopback**, which can be selected from the "Overall controls" menu accessible from the "Edit" Menu on PeakSimple's main screen. Make sure that the "Sample rate" is set to 5Hz.

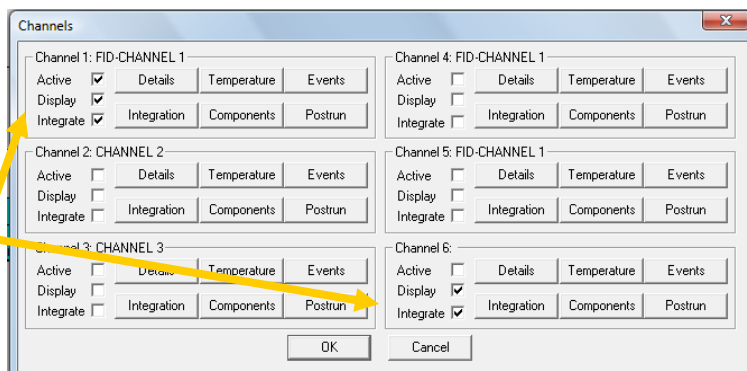


The 'Overall controls' dialog box in PeakSimple software contains various settings for the instrument. Key settings include:

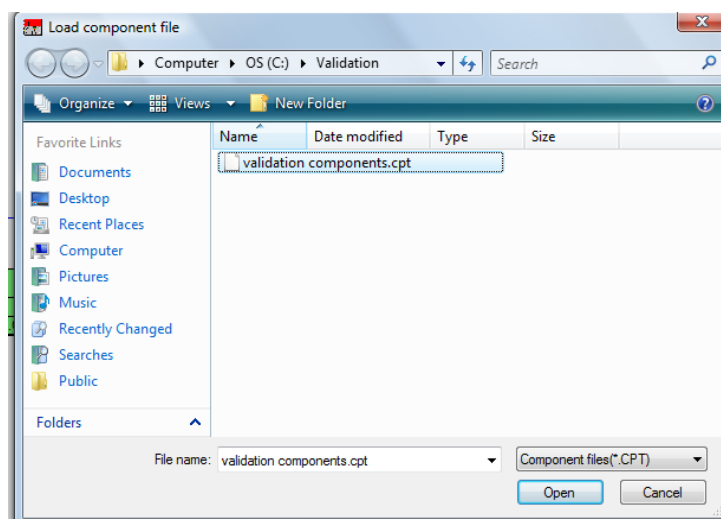
- Unknown peaks are labelled:** (empty field)
- Show retention windows:** (checked)
- Board type:** 333 (1ch USB)
- COM Port / USB device number:** 1809
- Sample rate:** 5Hz
- Default display period:** Start: 0.000, End: 6.000
- Label peaks on screen by:** Name (checked), Retention time (checked)
- Gradient settings:** Min: 0.000 (V), Max: 1.000 (V)
- Graph labels:** Scale time by: 1.00, Decimal places: 3, Scale mV by: 1.00, Decimal places: 3
- Amounts below an MDL of 0.0 will be reported as:** N/D
- Default data file path:** (empty field)
- Reset relays at end of run:** (unchecked)
- Hardware loopback:** (unchecked)
- Software loopback:** (checked)
- Save files in both .ASC and .CHR formats:** (checked)
- Automatically save data every:** 0.0 minutes
- Save thumbnail images:** (checked)
- Main window title:** (empty field)

PeakSimple Software Self Validation

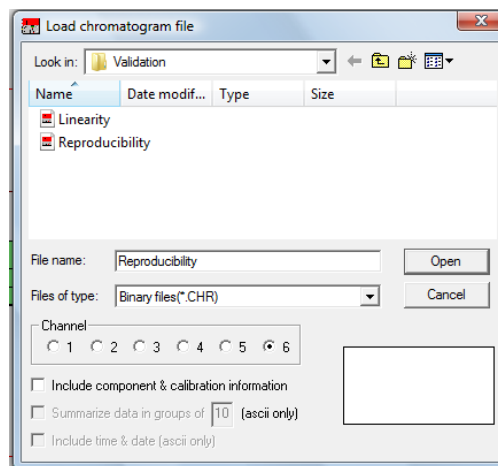
Initiate communications between PeakSimple and the GC or data-system. In the “Channels” Menu, make sure that Channel 1 is active, displayed, and integrated by checking the appropriate boxes. Ensure that Channel 6 is displayed and integrated.



From the main PeakSimple screen, right-click on Channel 1 and select “Components”. From the Components screen select “Load” and open the “Validation components.cpt” file from the C:\Validation file folder. Do the same thing for Channel 6.

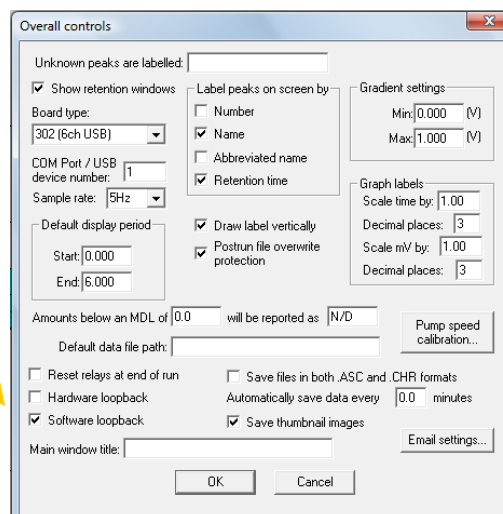


Load the “Reproducibility.chr” chromatogram into Channel 6 by selecting “Open” from the File menu, selecting the “6” Channel button, and selecting the Reproducibility.chr file from the C:\Validation folder. Hit the Open button.

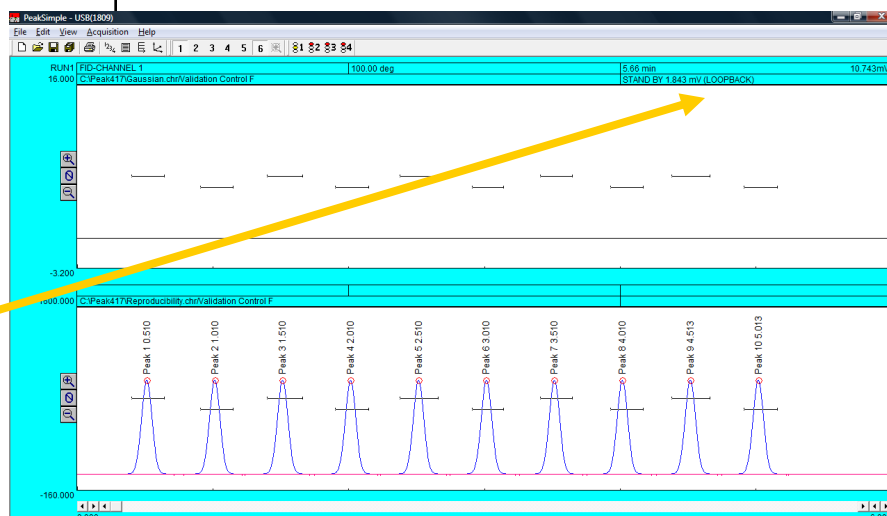


PeakSimple Software Self Validation

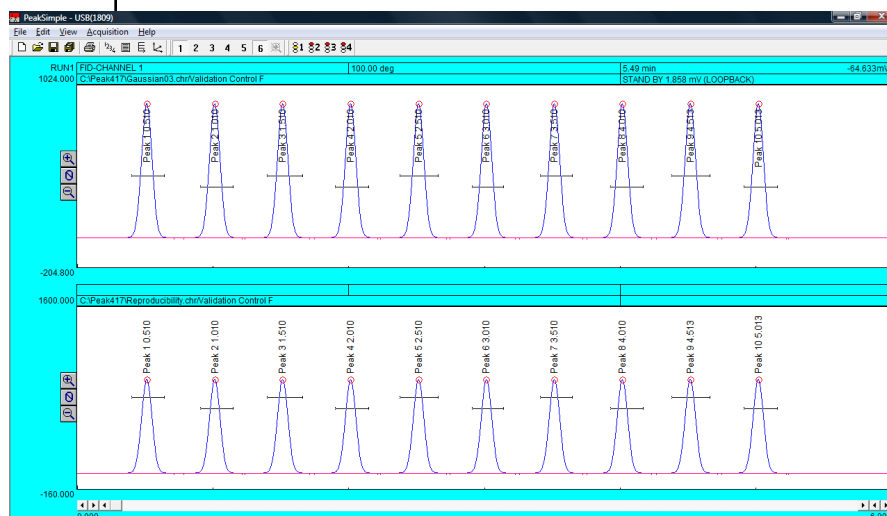
In the Overall Controls menu select "Software loopback" and hit the OK button. Software loopback will take whatever chromatogram is in Channel 6 and reproduce it in Channel 1. The data is transferred bit for bit in real time just as if Channel 1 is acquiring new data.



Your PeakSimple screen should look like this. Notice the "(LOOPBACK)" next to the signal display in the upper right hand corner of the screen.



Start the Validation run by selecting "Run" from the Acquisition menu or press the Spacebar on your keyboard. At the end of the run your screen will look something like this.



PeakSimple Software Self Validation

Once the run is completed compare the results of Channel 1 to Channel 6 in order to see how faithfully the data was reproduced. In this instance, the area counts of all the peaks are identical.

Component	Retention	Area	Height
Peak 1	0.510	5002.1034	898.162
Peak 2	1.010	5002.1086	898.633
Peak 3	1.510	5002.2028	899.073
Peak 4	2.010	5002.1536	899.420
Peak 5	2.510	5002.2016	899.552
Peak 6	3.010	5002.3356	899.352
Peak 7	3.510	5002.2496	898.950
Peak 8	4.010	5002.0976	898.491
Peak 9	4.513	5002.0056	898.180
Peak 10	5.013	5002.3102	898.654

Component	Retention	Area	Height
Peak 1	0.510	5002.1034	898.162
Peak 2	1.010	5002.1086	898.633
Peak 3	1.510	5002.2028	899.073
Peak 4	2.010	5002.1536	899.420
Peak 5	2.510	5002.2016	899.552
Peak 6	3.010	5002.3356	899.352
Peak 7	3.510	5002.2496	898.950
Peak 8	4.010	5002.0976	898.491
Peak 9	4.513	5002.0056	898.180
Peak 10	5.013	5002.3102	898.654

In order to calculate statistically meaningful measurements (i.e. standard deviation), several validation runs may be required. To simplify the process, the user can automate the validation runs by opening up the "Postrun" menu from the Channels menu. In the Postrun menu ensure that the "Save file as" box is checked and given a name and the "Auto-increment" box is checked. Check the "Add to results log" box and give it a name. Finally, check "Restart run after" and enter a time and the number of runs that you would like to have it perform. The data from the runs will be saved to the .LOG file where it can be viewed or easily exported to a data management program like Excel.

Channel 1 post-run actions

☒ Save file as: Gaussian03.chr ☒ Auto-increment

☐ Or use list of filenames: List

☐ Save results ☒ Add to results log: CH1.LOG

☐ Print results ☐ Update DDE link ☐ Save picture

Execute:

☒ Restart run after: 0.50 minutes 10 times total (9 remaining)

☐ Recalibrate at level: 1 ☐ Save results file to FTP site

☐ Smooth first ☐ Save data file to FTP site

☐ Copy data to channel: 1

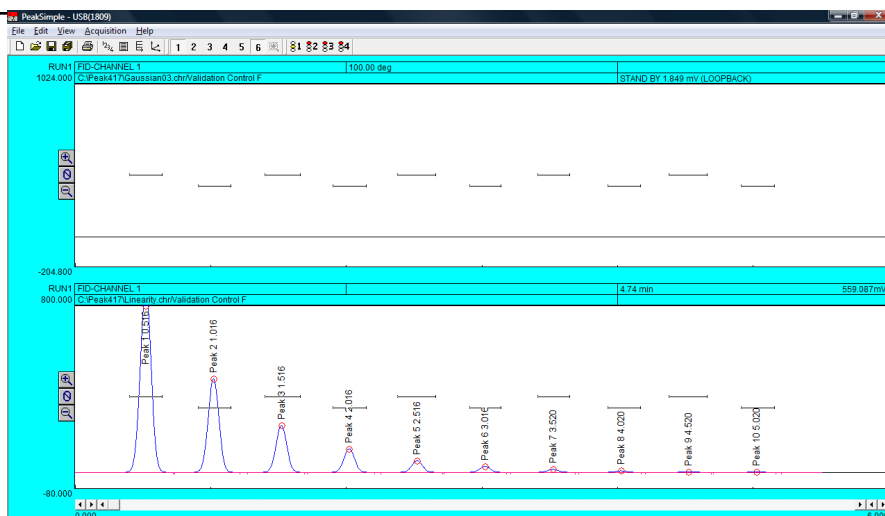
☐ Add to 3D display

Email: ☒ No ☐ On alarm condition ☐ Always

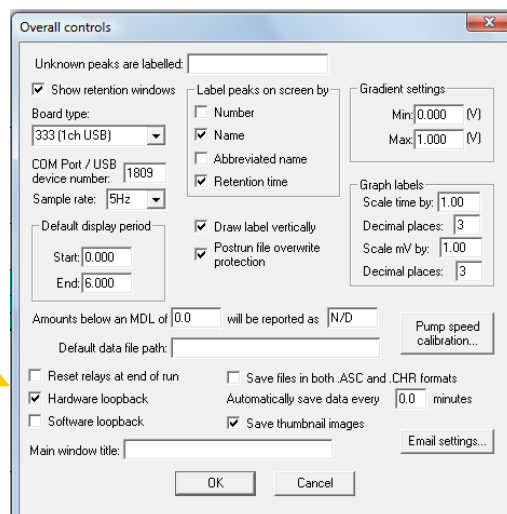
OK Cancel

PeakSimple Software Self Validation

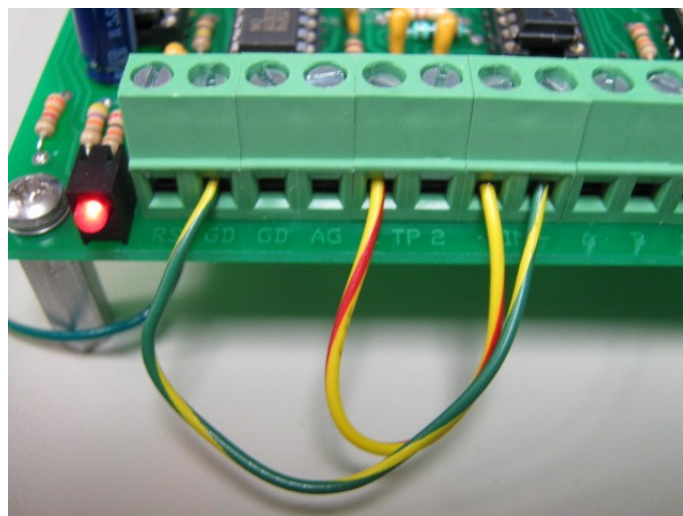
To test for linearity rather than reproducibility, simply perform the same process as previously outlined, except this time load the "Linearity.chr" file into Channel 6. For this chromatogram each succeeding peak has half the area counts of the one before it. When you do this the PeakSimple screen will look something like this.



To perform Hardware loopback validation select "Hardware loopback" from the "Overall controls" menu. In general, Hardware Loopback will have more deviation than Software loopback due to a difference in resolution (14 bits for Hardware, 24 bits for Software). With Hardware loopback the chromatogram in Channel 6 is played back as an analog voltage which Channel 1 re-acquires just like a real chromatogram.

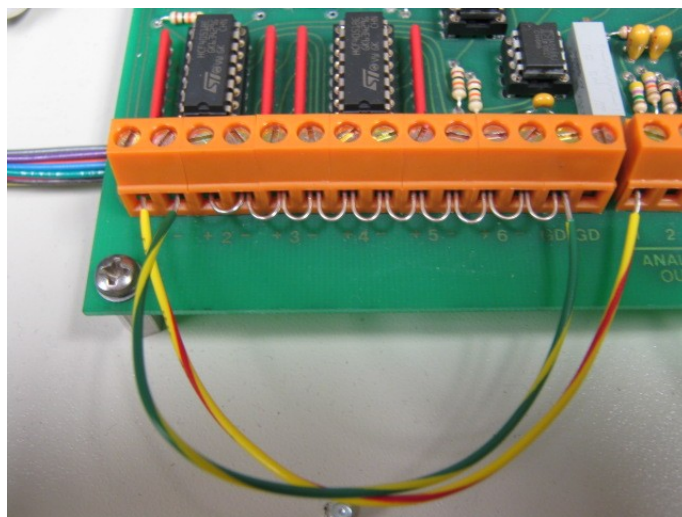


If you have a 333 single channel data system (or board inside your GC) connect a wire from ground to the negative signal input terminal, and another wire from the TP 1 terminal to the positive signal input terminal. It should look like the picture to the right.



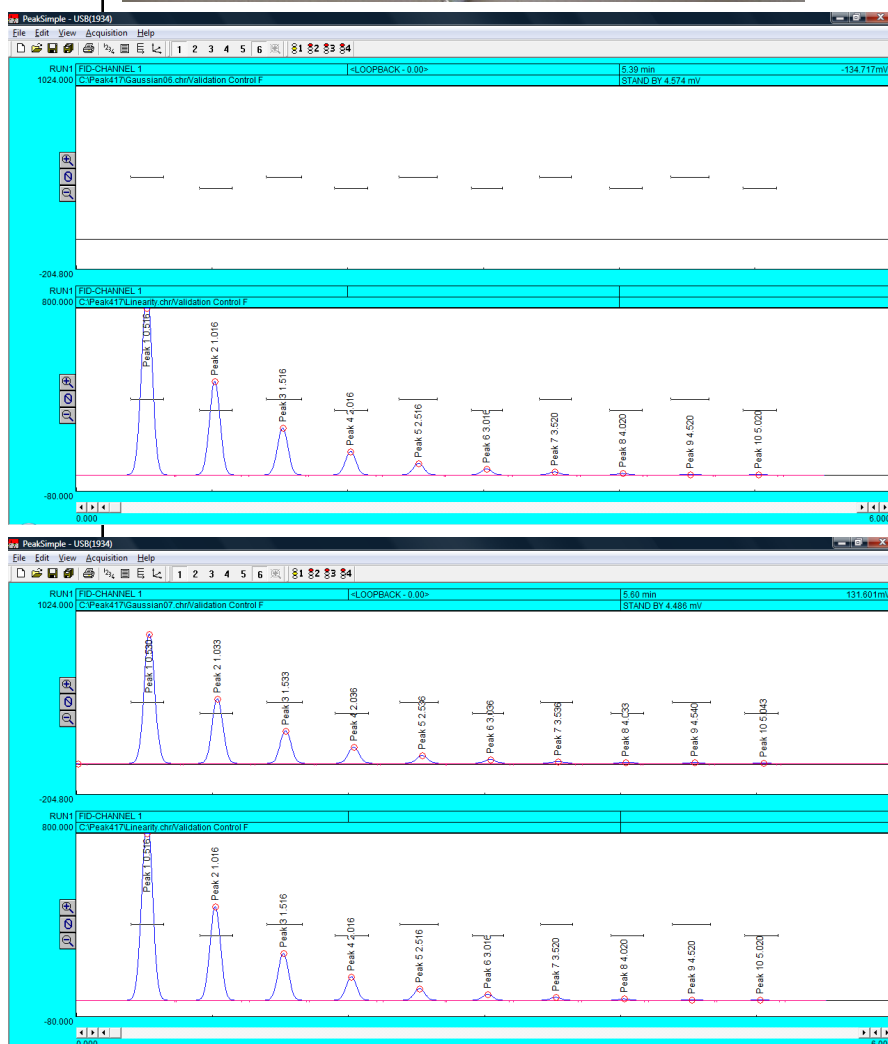
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If you have a six-channel 302 data system (or board inside your GC) connect a wire from ground to the negative channel one and another wire from the 1 analog out terminal to the positive channel one terminal. It should look like the picture to the right.



With the Validation components file loaded into Channels 1 and 6 and either the Reproducibility or Linearity chromatogram loaded in channel 6 (in this case Linearity is loaded) start the run.

When the run is completed compare the area counts between the two channels. As discussed previously, you can automate a number of validation runs in order to collect statistical information.



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The Reproducibility.chr and Linearity.chr chromatograms are very clean and easy for the software to integrate. It may be beneficial and more realistic to use your own chromatogram in order to obtain your validation data. In this instance, load a chromatogram of your choosing into Channel 6 and perform Software loopback or Hardware loopback as discussed previously.

Make sure to add retention windows over the peaks (see the PeakSimple tutorial for adding retention windows), save the resulting component file, and load it in channel 1. This will allow you to quantify the area counts of your peaks after each validation run.

For any validation runs, print the chromatograms in order to have a hard copy of your data.

