5. Chromatography Data System

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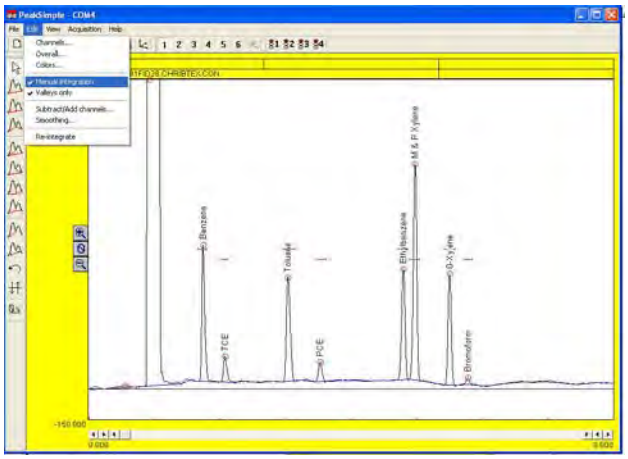
Pull Down Menus

All PeakSimple for Windows features may be accessed from pull-down menus. When you click on a menu bar item, a pull-down group menu will open to permit navigation to specific group features.



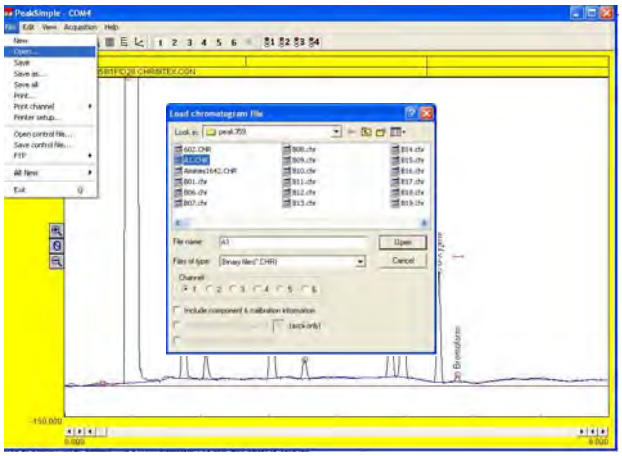
FILE Pull-Down Menu

NEW

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

OPEN

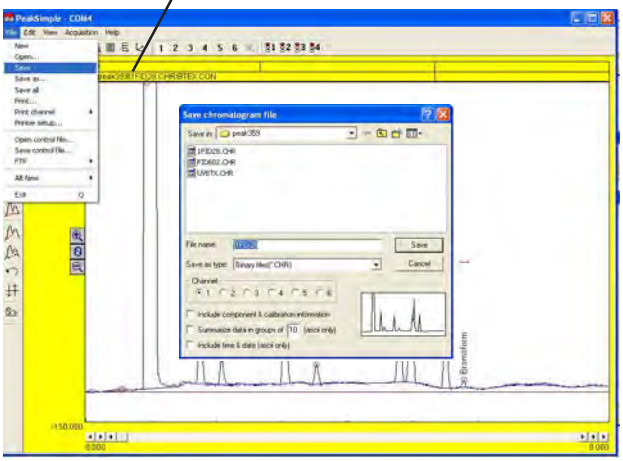
To open a previously saved chromatogram file, select **FILE-OPEN. A LOAD CHROMATOGRAM FILE** screen will appear which will allow you to select any file from any directory (folder) on your system. Choose the channel (1-6) in which you wish to display your saved chromatogram and then click **OPEN.**



Filename

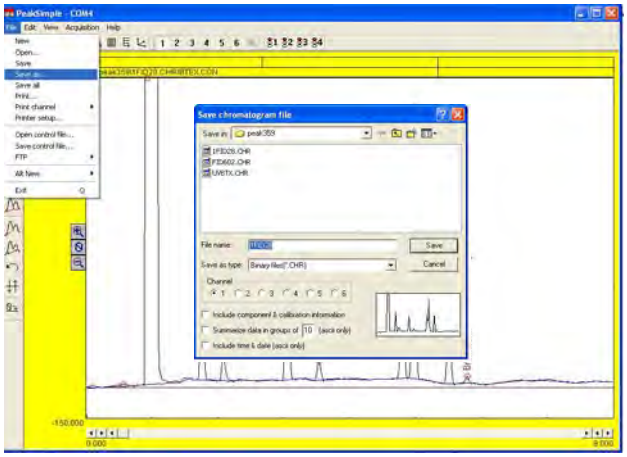
SAVE

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



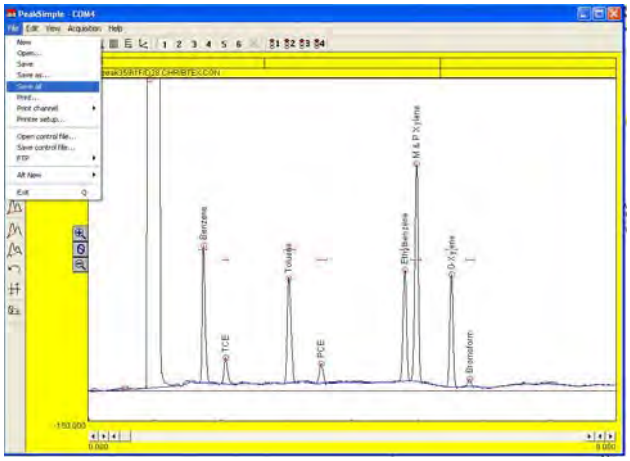
SAVE AS

To save a newly created chromatogram file, select **FILE-SAVE AS. A SAVE CHROMTOGRAM FILE** screen will appear which will allow you to safe the file in any directory (folder) on your system. Type a name into the **File Name** box and choose which channel (1-6) you wish to save and then click **SAVE.** The file will be saved as a **binary file** by default, with a **.CHR** extension. You may also select to save the file in **ASCII** format with a **.ASC** extension.**FILE-SAVE** feature saves the displayed chromatogram.



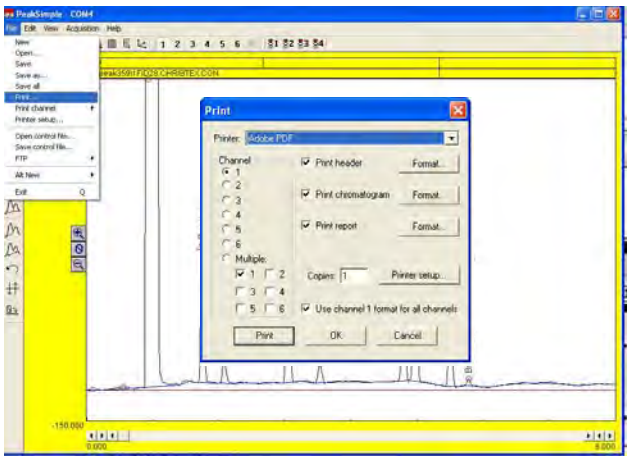
SAVE-ALL

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



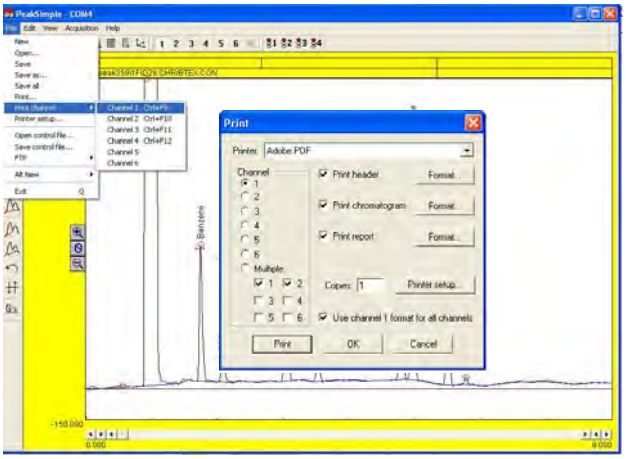
PRINT

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



PRINT - Channel 1

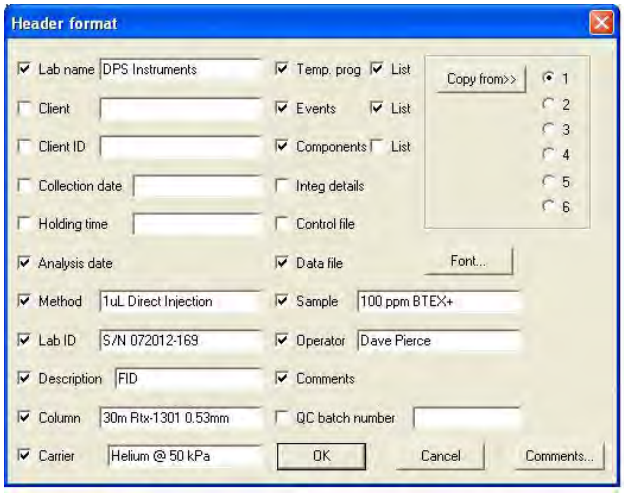
When you access the **FILE-PRINT** pull-down menu you will notice that you can select to print any combination of **multiple** channels by clicking on the circle next to the word **multiple**. You may also choose to print individual channels by clicking on the circle next to the desired channel. **Click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



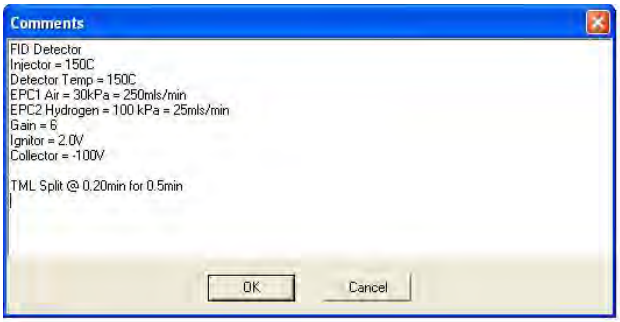
PRINT HEADER FORMAT

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

Print out **Temperature Programs, Events and Components** file names by checking their boxes; or click on **List** to print the complete Temperature Program, Event Table of Component List. **Copy from:** selects which channel will provide the **List** information.

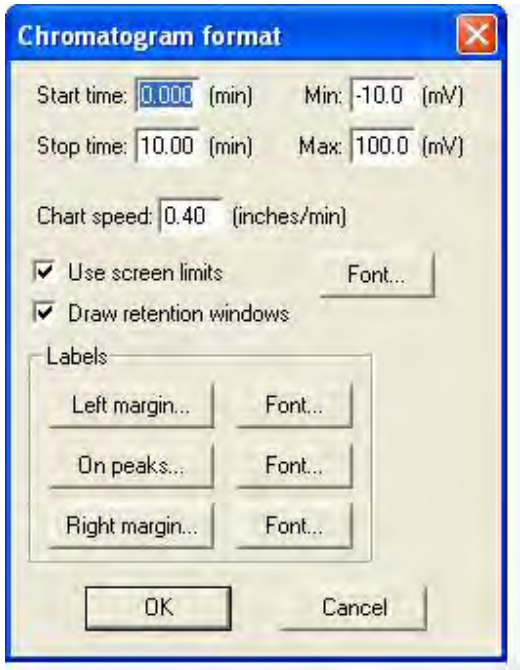


Check the **Comments** box and click on **Comments...** to enter customized information about your analysis. You can change the **Font**, style and size of your printed text by clicking on the **Font** box. Select a size that will provide readable text while still leaving room for your chromatogram and report. Then you access the **FILE-PRINT** pull-down menu **FILE-SAVE-ALL**



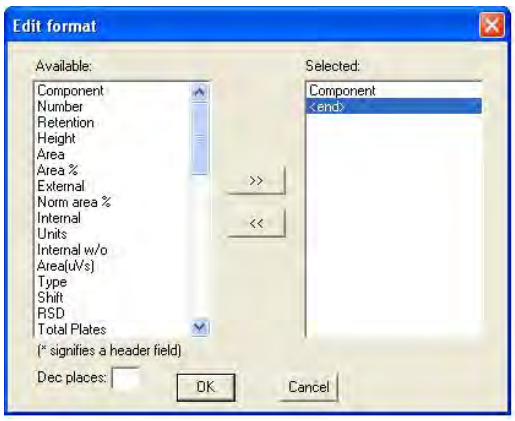
PRINT CHROMATOGRAM FORMAT

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

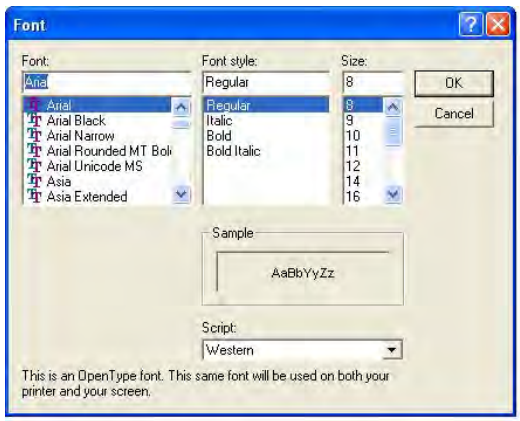


The **Chart speed** setting will determine the size of the chromatogram section of your printout. A setting of **1.0 inches/minute** for a 5 minute chromatogram will produce a **5 inch** chromatogram print. You may need to experiment with the settings to fit your **header, chromatogram and report** information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

The **Labels** section of the screen lets you select what useful information will be printed along the borders of the chromatogram, and above the peaks. Clicking of **On Peaks**, for example, will bring up the **Edit format** screen which will allow you to select from a list of measurements which will automatically be calculated and printed on the peak of your chromatogram.



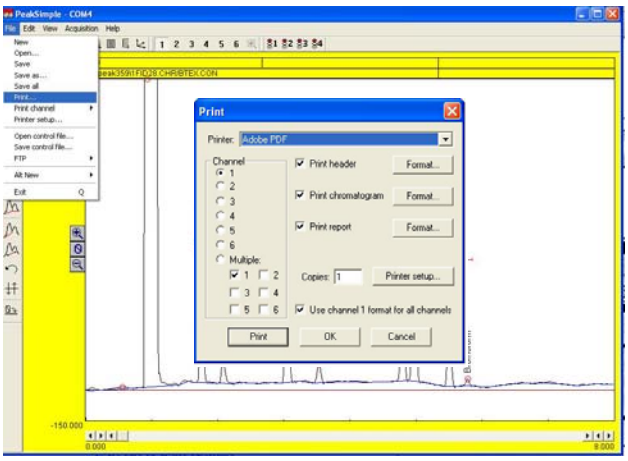
To choose **Component**, for example, click on **Component** from the left column and then click on the right arrows (>>). **Component** will now appear in the **selected** column on the right. Click **OK** to close the window.



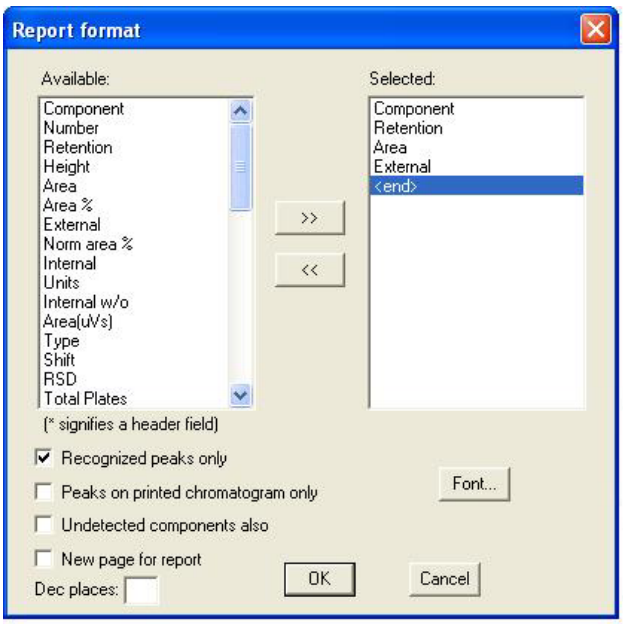
You can change the **Font**, style and size of your printed text by clicking on the **Font** box. Select a size that will provide readable text while still leaving room for your chromatogram and report.

PRINT REPORT FORMAT

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



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

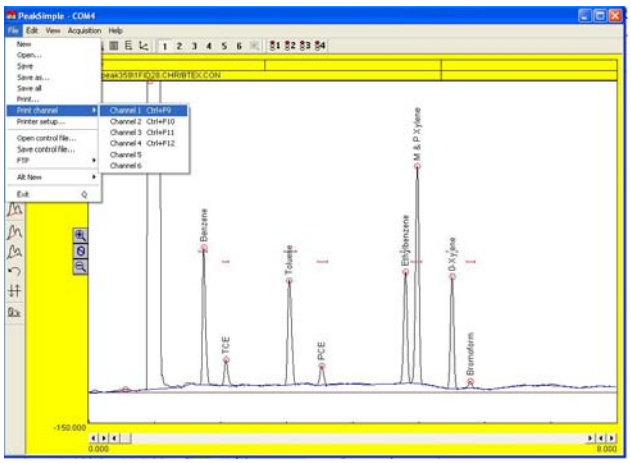


Clicking on the box next to **Recognized peaks only** will place a check mark in the box and only those peaks which integrate properly within named retention windows will be printed in the report. Checking the **Peaks on printed chromatogram only** box will allow the report to show only those peaks defined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

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

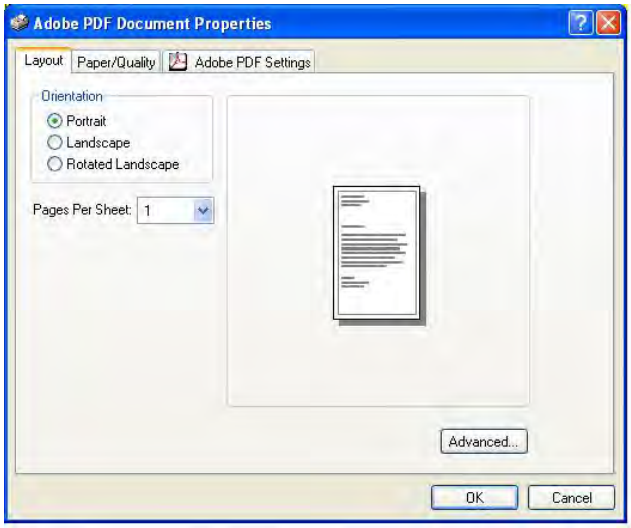
PRINT CHANNEL

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



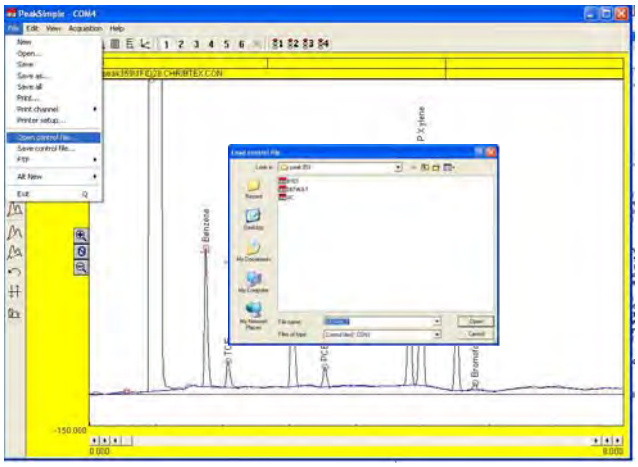
PRINTER SETUP

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



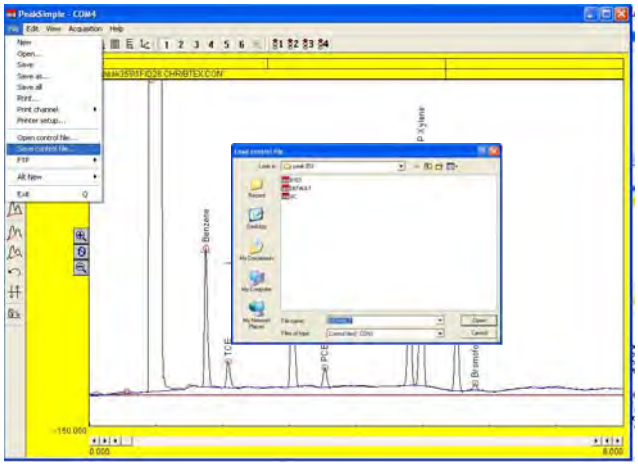
OPEN CONTROL FILE

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



SAVE CONTROL FILE

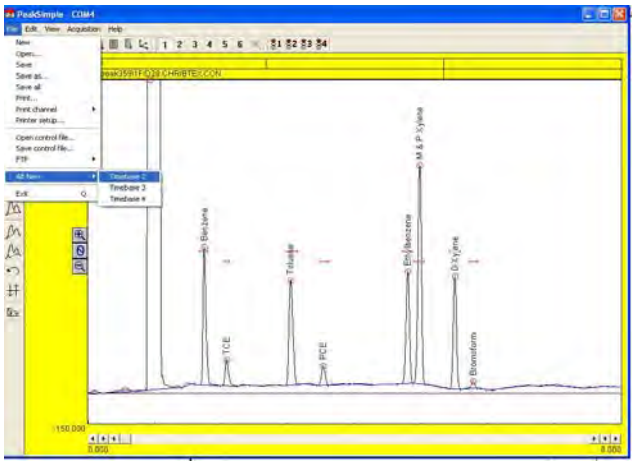
Once you have set up all of the user-definable parameters within PeakSimple for Windows that meet the requirements of your system and/or you specific analytic method, it is wise to save these settings for future use. PeakSimple uses **control files**, identified with a **.CON** extension, to save the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



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

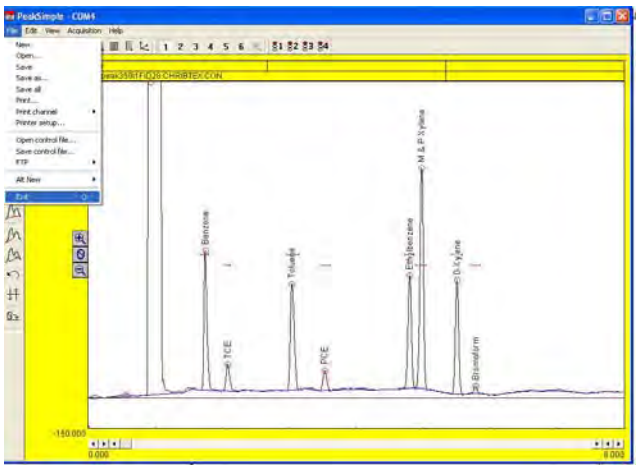
ALT NEW

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



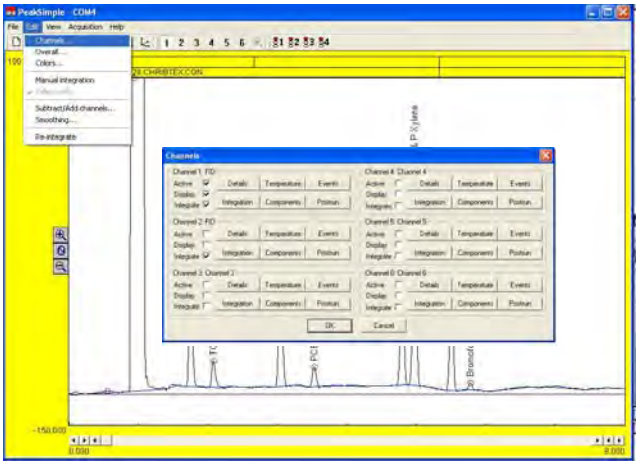
EXIT

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

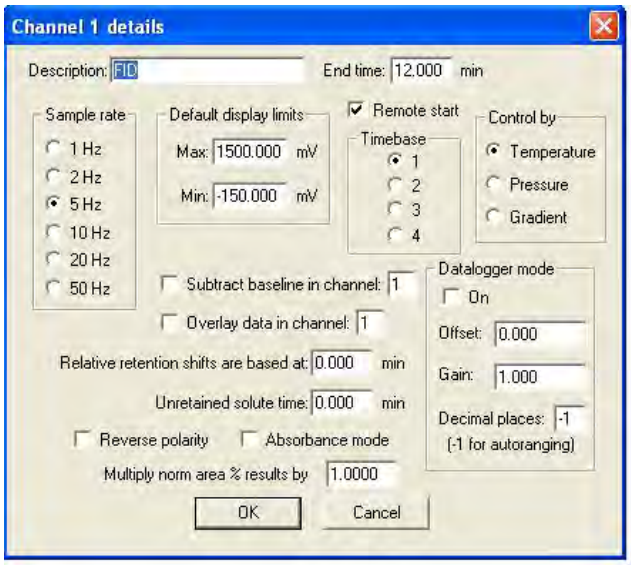


EDIT Pull-Down Menu

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



CHANNELS DETAILS



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

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

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

The **Remote Start** feature allows the user to start a chromatographic run using an external signal such as a autosampler. Check the box to enable **Remote Start.**

Unretained Solute Time

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

Timebase

The **Timebase** selection assigns the channel to a trigger group. The software can trigger four separate chromatographs, however we only use Timebase 1. Any **Channel** with the Timebase trigger group selected will start running when the **SPACEBAR** is pressed and end when the **END** key is pressed.

Temperature, Pressure, Gradient, Absorbance

The Temperature button is used for GC analysis, the other buttons are used for HPLC analyses.

Datalogger

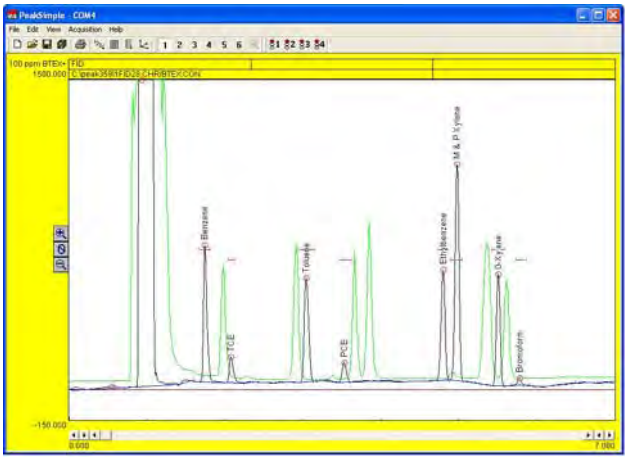
The datalogger button will display just the mV signal in the chromatogram section. This is used to monitor the change in detector signal when no column is present, such as a Total Hydrocarbon analysis, where the sample bleeds directly into the detector.

Subtract Baseline in Channel "X"

Checking **Channel 1**'s box for **Subtract Baseline in Channel "X"**, where **"X"** is 1,2,3,4,5 or 6, will cause the chromatogram in **Channel 1** to subtract the baseline stored in **Channel "X"**, while running in real-time. Load the baseline to be subtracted into an inactive channel to ensure that the data is not deleted by the start of a new run on that channel. (Uncheck the **active** box, see **Edit-Channels**). Baseline subtraction can also be performed using PeakSimple's **Edit-Subtract/Add Channels** feature, however, this is not a real-time function, but a post-run function, done at the end of the chromatographic run.

Overlay Data in Channel "X"

Checking **Channel 1**'s box for **Overlay Data in Channel "X"**, where **"X"** is 1,2,3,4,5 or 6, will overlay the data stored on **Channel "X"** onto **Channel 1** using contrasting colors. The channel selected for overlay can be either an active or inactive channel. When the overlay channel is active then the overlay will be seen in real-time.

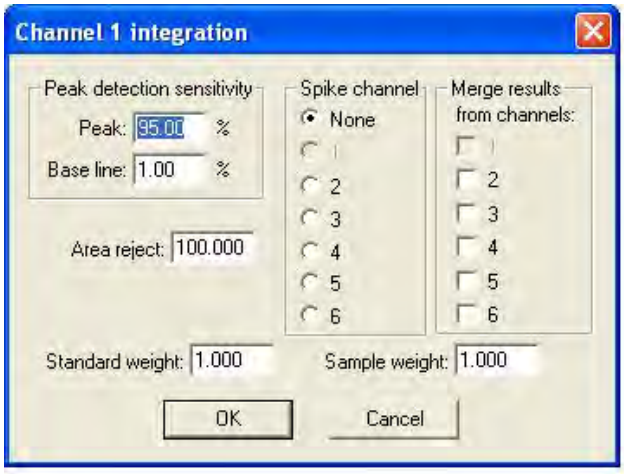


Relative Retention Shifts Are Based At "X" Minutes

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

CHANNELS-INTEGRATION

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



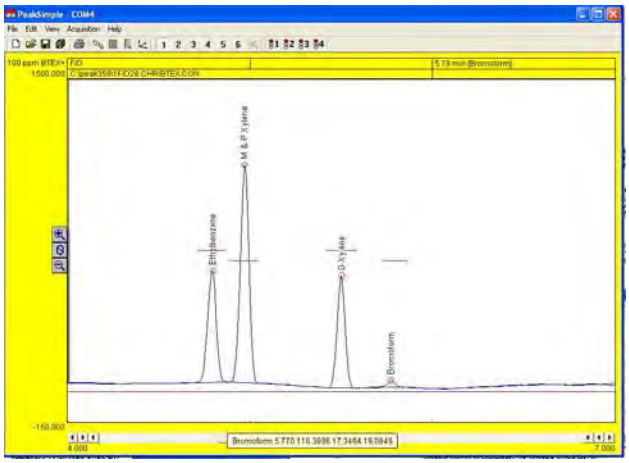
Peak Detection Sensitivity

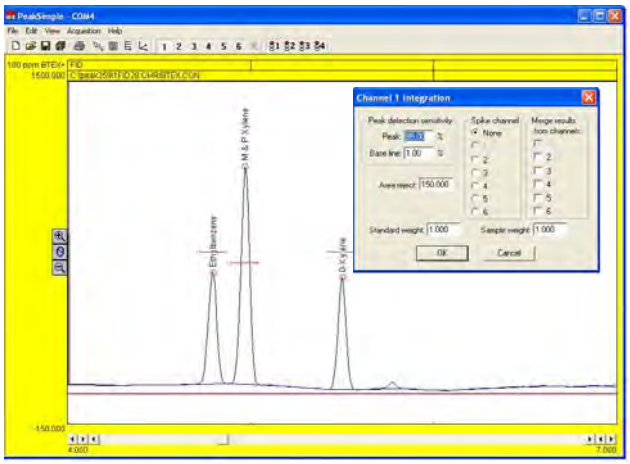
The **Peak** sensitivity setting determines how PeakSimple detects the beginning and end of a peak. A high **Peak** number requires only a small slope change to initiate the start or end of the peak. A low **Peak** number requires a very large slope change to initiate the start or the end of the peak. We typically set the value to 95.

The **Baseline** sensitivity setting determines how PeakSimple attaches the baseline to the data line. The larger the **Baseline** number; the more likely PeakSimple will draw the baseline to a valley between two peaks. The smaller the **Baseline** number; the more likely PeakSimple will drop a vertical line from a valley to a horizontally constructed baseline below the peak. We typically set the value to 1.

Area Reject

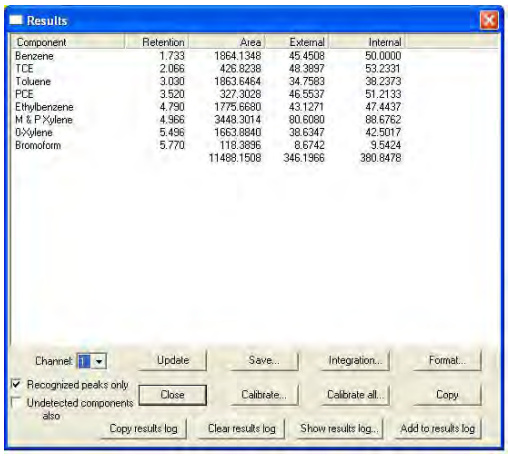
If a chromatogram contains peaks whose area counts fall below the threshold defined by the **Area Reject** for that channel, the peak will be ignored and no integration will occur. If the peak area is of interest, you can lower the **Area Reject** value until the peak in question is integrated. Integrated peaks are marked with a circle at the top of the peak. In the example below Bromoform has an area of 118, if the Area Reject is increased to 150, bromoform is no longer integrated.

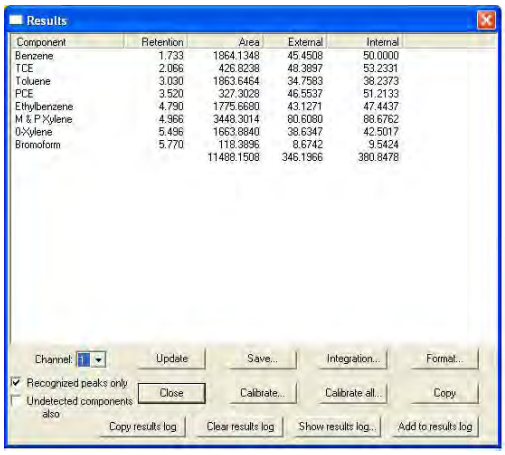




Standard Weight

PeakSimple for Windows determines the internal or external standard results by the ratio of the STANDARD divided by the SAMPLE. The **Standard Weight** setting maybe changed to adjust the channel's quantification, affecting internal or external peak results by the factor entered. For instance: A setting of 2.000 will double the weight of the standard thereby doubling the internal or external standard results.



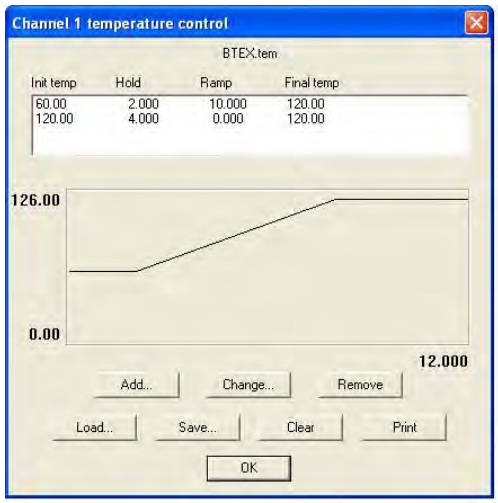


Sample Weight

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

Spike Channel

Another feature of PeakSimple for Windows allows you to display the results of a matrix **Spike Channel** subtraction.



EDIT-CHANNELS-TEMPERATURE

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

Temperature Segment Details

Add Button

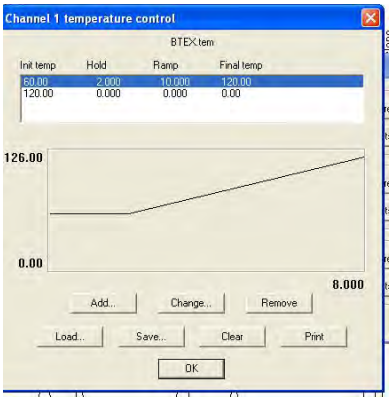
Click on the **Add** button from a blank **channel 1 temperature control** window to create a new temperature program for column oven #1. Type the required data in the following fields: **Initial temperature**, the **Hold** period in minutes, the **Ramp** rate in °C / min and the final **Temperature**, or the duration of the Ramp.

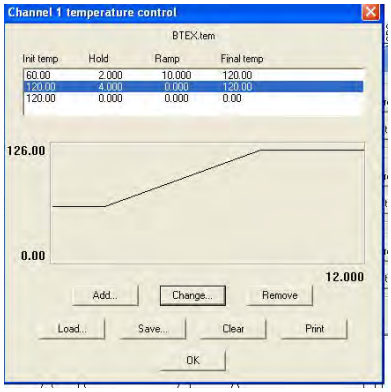
The length of the run is automatically calculated by PeakSimple based on the information provided in these fields, and is also displayed in the **EDIT-Channel-Details End Time** field. Additional ramp segments may be added by clicking **Add** button again.

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

Change Button

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



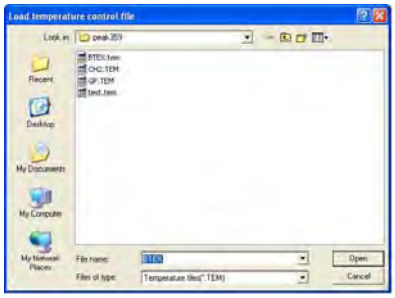


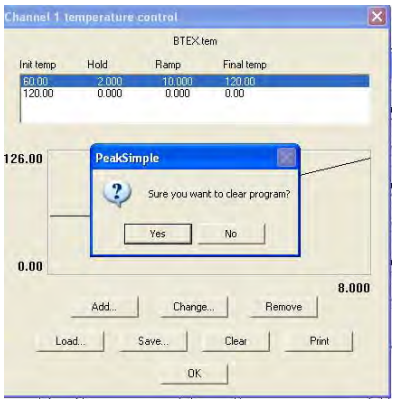
Remove Button

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

Load Button

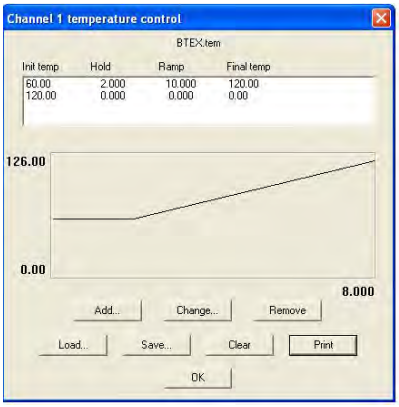
Click on the **Load** button to load an existing temperature control file, or to update an existing one. Remember to use the **.TEM** extension when naming the temperature control file. The saved file name appears at the top of the temperature control window indicating the file in use.





Clear Button

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

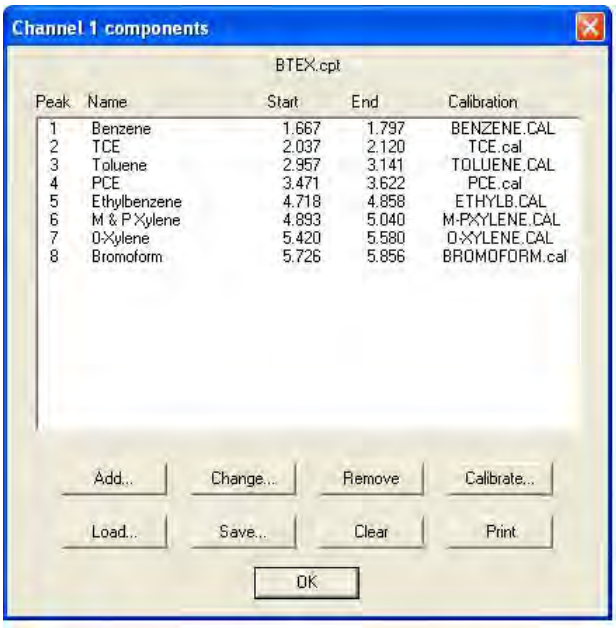


Print Button

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

CHANNELS-COMPONENTS

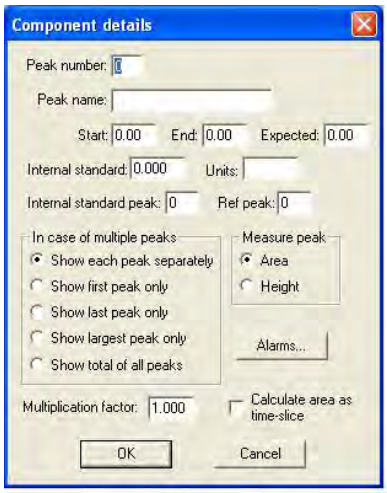
PeakSimple for Windows can identify and quantify sample components through the use of a component table. The component table enables PeakSimple to recognize each peak by its retention time and compare the area counts against the calibration curve to produce actual concentration data. The user can edit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

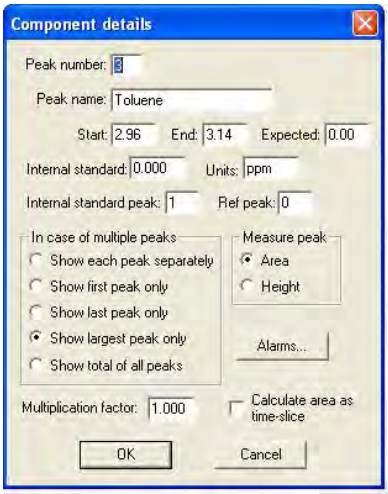


When a component table is loaded, the table will show each component by its peak number, peak name, the start time for the retention window, the stop time for the retention window, and the associated calibration file name. Different component tables may be used for each active channel and any component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

COMPONENT DETAILS

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



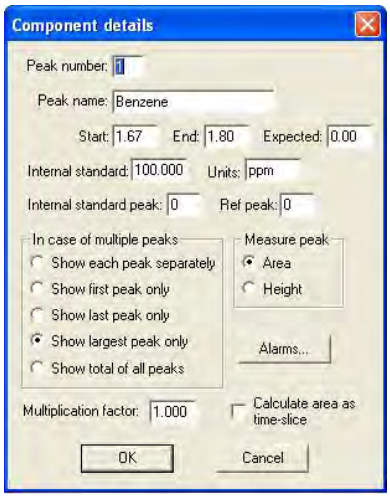


Peak Number, Peak Name, Start and End

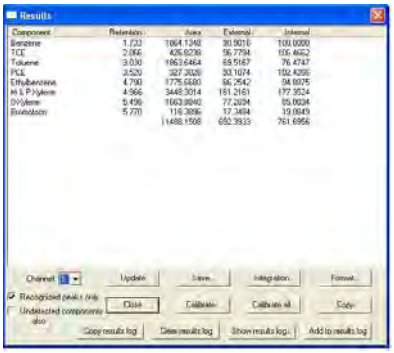
A blank **Component Details** screen is opened by selecting the **Add** button. Enter a unique **Peak Number** for each component, typically starting with 1 and incrementing for each additional peak. Then enter a unique **Peak Name** for each component. **Start** and **End** define the beginning and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

Internal Standard and Units

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

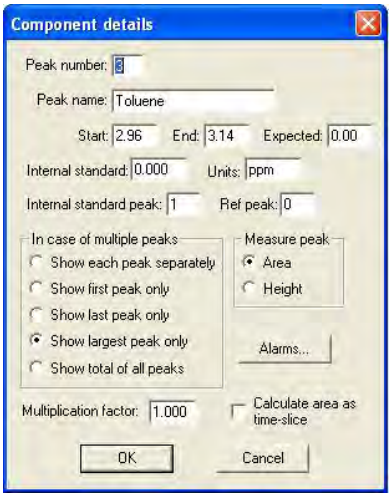


The **internal standard** calculation yields a result which is the **external result times the ratio of the know concentration of the internal standard peak divided by the external result for the internal standard peak.** As shown in the example to the right, note that while the external result for Benzene yields exactly 100 (the known concentration) as a result of the calculation **90.90 x 100/90.90.** In the same way, the internal result for every analyte peak which is referenced to Benzene is calculated as **external result x 100/90.90 = internal standard result.**

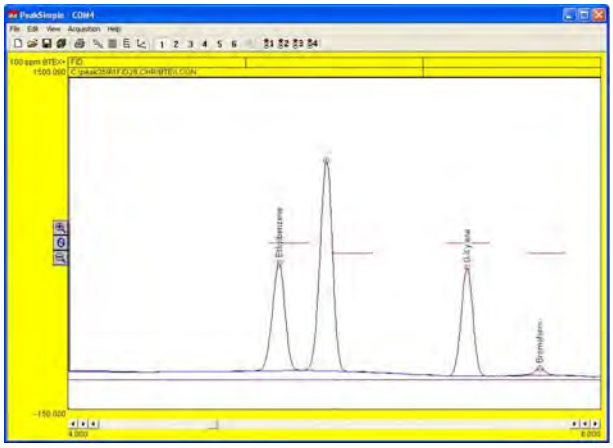


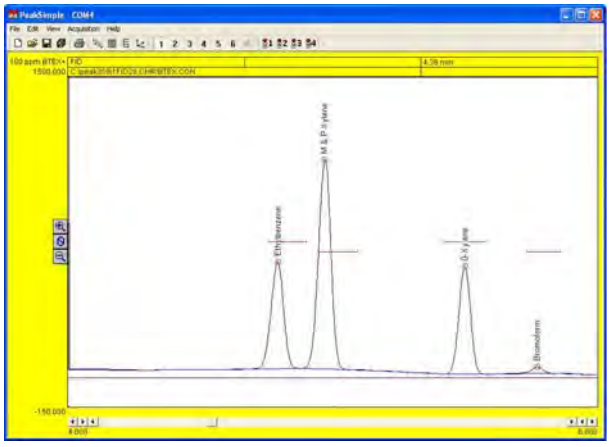
Internal Standard Peak

Peaksimple allows any peak to be referenced to any other peak for internal standard calculations. Typically all analyte peaks will be referenced against a single **Internal Standard Peak.** In this example Toluene is referenced to Benzene (Peak #1) by entering 1 in the **Component Details** screen dialog box labeled **Internal Standard Peak.** Notice that the **Results** screen (**View Results**), will reflect the new value for all peaks' internal results.



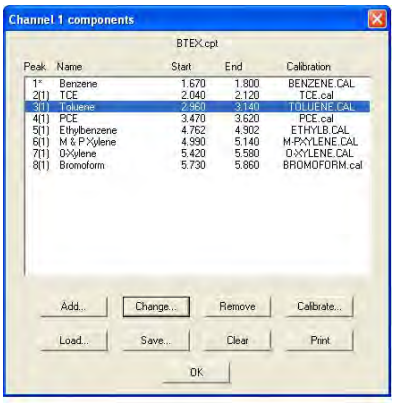
A Reference Peak is used to shift the retention windows of other peaks. In the example below, M&P-Xylenes eluted prior to their retention window and were not integrated. By entering a value of **5** in the **Reference Peak** box, M&P-Xylenes retention windows are referenced to ethylbenzene, (peak #5). M&P-Xylenes retention window is then shifted by a percentage equivalent to chlorobenzene's distance from the middle of its retention window. This shift in the ethylbenzene retention window allows M&P-Xylenes to be integrated.

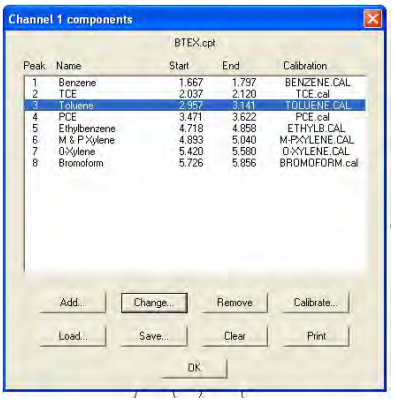




Change Button

Click on an existing component to select it. Click on the **Change** button to change the parameters of the component.



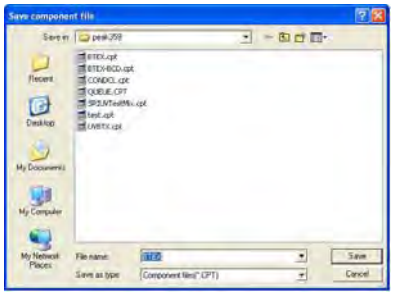


Remove Button

Click on the **Remove** button to remove the component from the component table.

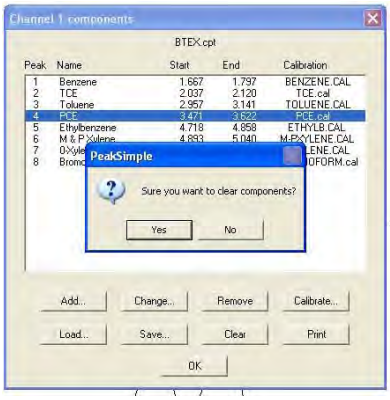
Load Button

Click on the **Load** button to load an existing component file, designated with the **.CPT** file extension.



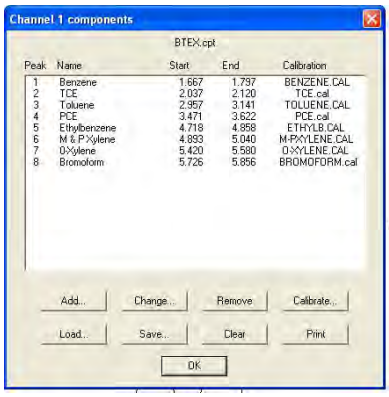
Save Button

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



Clear Button

Clicking on the **Clear** button deletes all component data from the component window. The component file name is also removed.



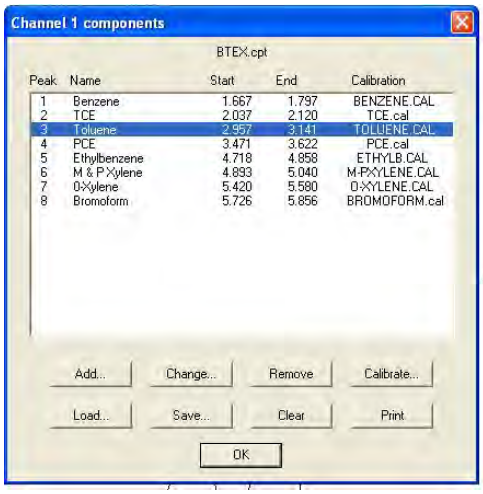
Print Button

Clicking on the **Print** button sends the file data and the component table information to the printer.

Calibrate Button

After creating a component table, each component in the table will need to be calibrated. This allows PeakSimple for Windows to not only identify each analyte peak, but also to quantify each use peak using a calibration curve. 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

Inject a standard containing known concentration of the component you wish to calibrate. Use a concentration higher than what you would expect to encounter in your analyses. Another few samples should be run at lower levels, using precise dilutions of your standard. Make note of the area or peak height at each concentration or use the shortcut method described in the next section.

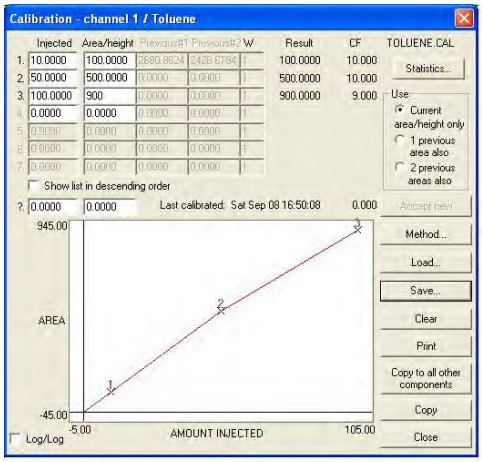


Calibration Window

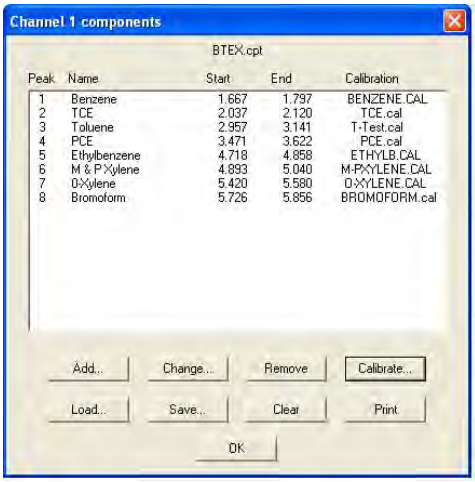
In the **Edit–Channels–Components** screen, highlight the component to be calibrated and select **Calibrate**. If this is the first time calibrating a component, an error message will appear which says "**Not enough data points**". This is simply a warning to inform you that PeakSimple currently does not have enough data points for the calibration method in use. Once enough data is entered for the calibration curve, this message will no longer appear. Click **OK** to bypass the error message and continue to the calibration window.

The **Calibration** will open and allow you to enter

the raw data that you previously obtained. In the example shown, data is entered into the table in the upper left corner of the calibration screen, beginning with the lowest concentration and ending with the highest concentration. If you wish to enter the data is descending order, check the **Show list in descending order** box. When entering data into the table, first enter the concentration injected, then the area count or peak height obtained.



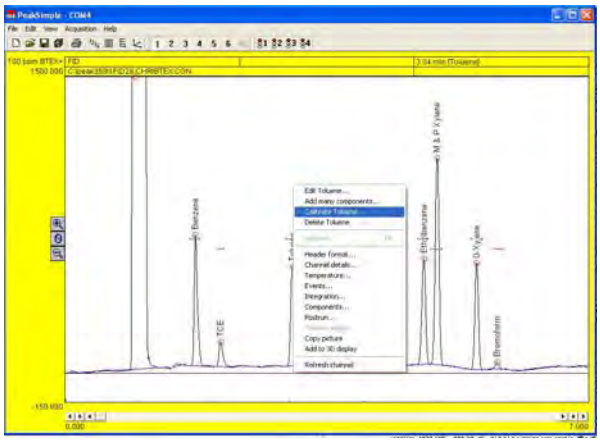
As data is entered for each concentration, a data point will be added to the calibration curve displayed in the lower screen of the window. You may use as many as seven concentration levels for your calibration curve. In the fictitious example on the right, a Toluene standard was injected in concentrations of 10 ppm, 50 ppm, and 100 ppm. The area counts from the FID detector were 100, 500 and 900, respectively. Notice the three corresponding data points on the newly created calibration curve.



When calibration for each component has been completed, click on the **Save** button to save and name the component's calibration file. Then click on the **Close** button to close the calibration window. In our example, a unique file named **T-Test.cal** was created. The T-Test.cal file name will now appear in the **Components** window next to Toluene.

WARNING:
Do not use the same calibration curve file name for two different channels or detectors since each detector requires its own calibration curve (ie BenzFID.cal; BenzPID.cal; etc.)

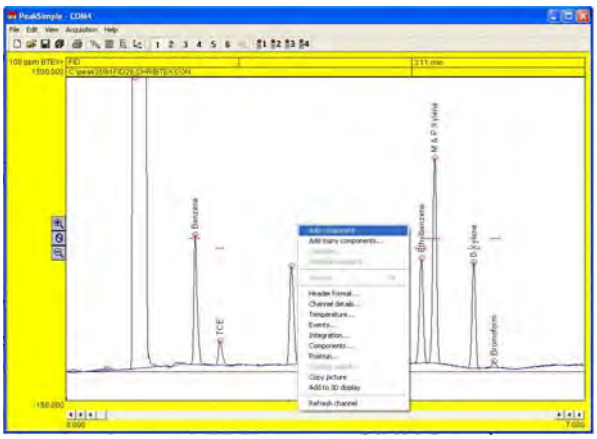
Calibration is required for each component you expect to be present in your sample, and for each detector you will be using in your analysis. Once calibration curves have been completed, and calibration files saved, every component in the component table should show an associated calibration file. PeakSimple will now be able to quantify each component when actual samples are injected.



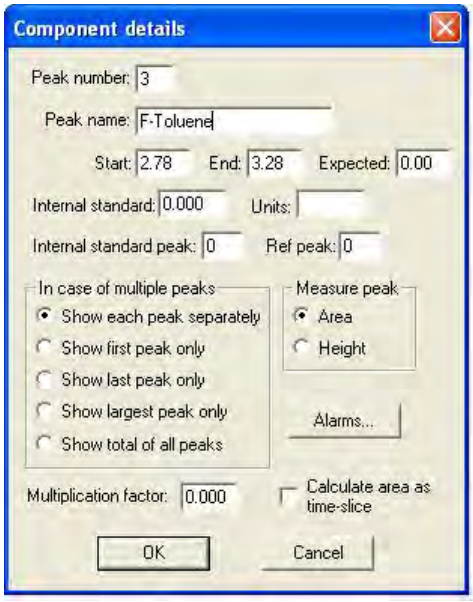
Calibration Screen Shortcuts

As an added convenience, PeakSimple for Windows offers shortcuts to commonly used screens. These shortcuts may be accessed by pointing to the peak on the desired channel and clicking once on the **right** mouse button. The following pages describe the shortcuts available to set up calibration tables and calibrate components.

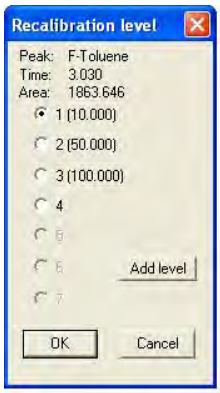
After a know standard has been run and peaks have been identified, a new component table may be constructed by simply positioning the mouse pointer over a peak clicking once on the right mouse button, ("right-clicking"). The shortcut menu will appear. Select **Add component** from the menu. A retention window will be drawn horizontally across the peak.



Right-click again over the peak and select **Edit component.** The **Component details** screen will open allowing the peak to be named and numbered. The example below shows Toluene as peak #3 The component has been named F-Toluene to avoid confusion with a toluene peak from another detector such as a PID.



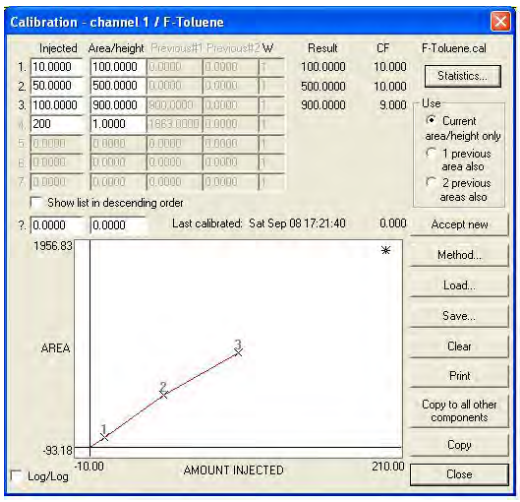
Note: It is important that you choose the component name carefully since the calibration file name is derived from the component name. The F-Toluene calibration file would be named F-Toluene.cal.



Right-click over the peak again and select **Calibrate.** If no calibration curve exists for the peak, a window will open asking if you would like to use a calibration file. PeakSimple offers a template calibration file aptly named TEMPLATE.CAL. Click **yes** to use the default TEMPLATE calibration file or select your own by clicking **Browse.** This example uses the template calibration file. Another window will open asking you to select the **Recalibration Level.** Select **100** for 100 ppm standards, **50** for 50 ppm, etc.

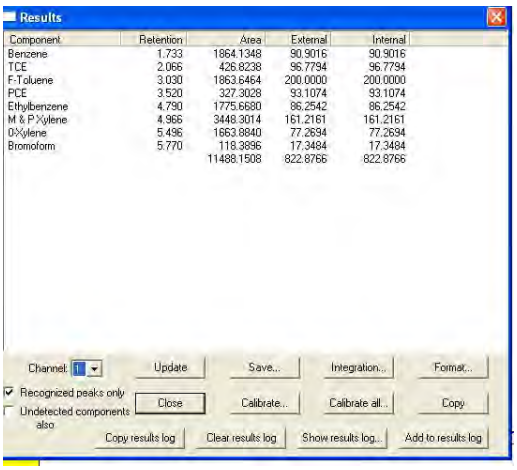
Click **OK** to accept the **Recalibration level**. The calibration screen will open and a flashing asterisk (*) will appear along the existing calibration curve depicting the new data point. Notice that the calibration curve has been named **F-Toluene.CAL**. If the new calibration data point is acceptable, click **Accept New** to update the calibration curve data.

In the example to the right the **F-Toluene.CAL** calibration table reflects the new area count of **1862** at the new concentration level of **200** ppm. At this point, if the new calibration curve data is deemed to be acceptable, click on **Close** to automatically save the new calibration file, and close the **Calibration** window.



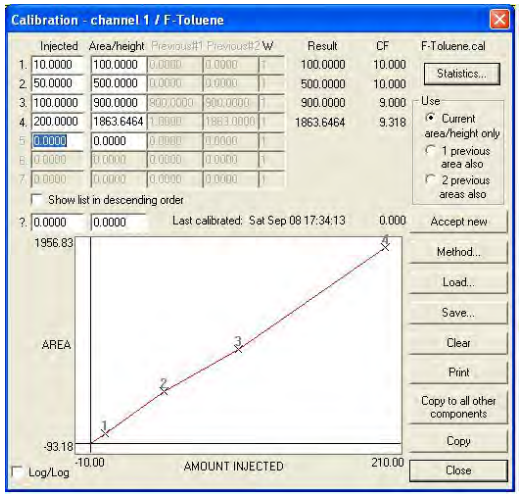
Calibrate All

PeakSimple offers a timesaving feature for **recalibrating all peaks** with just one mouse click. After a calibration curve has been created for each component, click on **View-Results** to bring up the result window. Select **Calibrate All** and choose an appropriate **Recalibration Level**, then click **OK**. PeakSimple will automatically recalibrate all components at the selected level and save each component's updated calibration file.



Calibration – Use and Statistics Radial Buttons

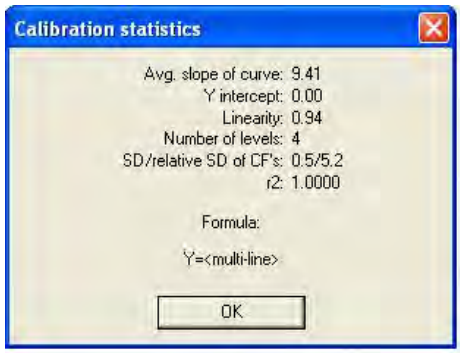
To improve the calibration accuracy, chromatographers may prefer to average the areas 1, 2 or 3 replicate injections. The **Use** radio button allows the user to select how many injections are used in the calculation of calibration factors (CF). Calibration factors are used to construct the calibration curve using the formula: CF = area count divided by the amount injected. The example to the right shows the calibration data at the 200 ppm concentration level, with the **Use** button set to the default setting of **Current Area / Height Only**. This setting uses only the latest calibration data to calculate the calibration factor for the #4 data point. (CF = 1863 / 200 = 9.318)



If you have injected multiple samples of the same standard, they can be averaged by setting the calibration to use **Previous Areas Also.**

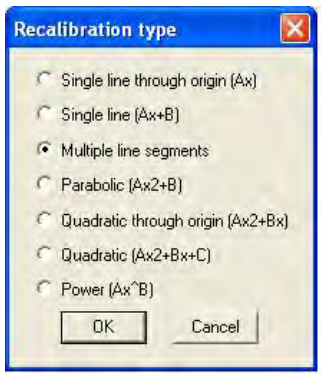
Setting **Use** to **2 Previous Areas Also** will average the last three areas to derive the calibration factor.

The **Calibration Statistics** screen shows calibration curve details such as the **Average Slope of the Curve**, the **Y Intercept**, the **Linearity** of the curve, the **Number of (calibration) Levels**, the **Standard Deviation and Relative Standard Derivation of Calibration Factors**, the **R2** and the **Formula** used which is based on the **Method** selected.

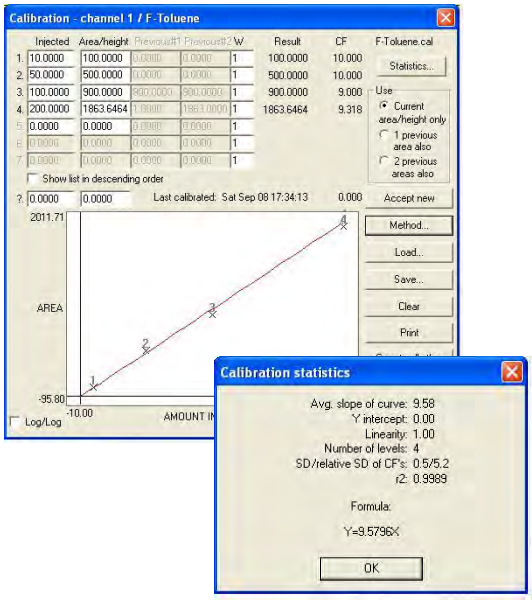


Calibration Window – Methods

The **Method** button opens the **Recalibrate Type** window which allows the selection of one of six formulas used to draw the calibration curve. The algorithms are described below and corresponding calibration statistics are shown.



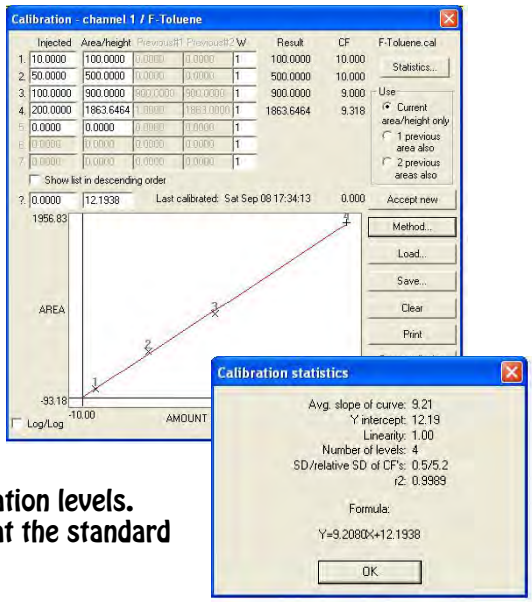
In the following:
X is the sum of the external measures over the calibration levels
Y is the sum of the corresponding areas at those calibration levels
n is the number of active calibration levels
Several other sums are used, for instance:
X2 is the sum of the squares of the external measures
Y4 is the sum of the (area to the 4th power)
XY is the sum of the (external measure *area)
X2Y is the sum of (external measure squared * area)
Y/X is the sum of the (area / external measure)
etc.



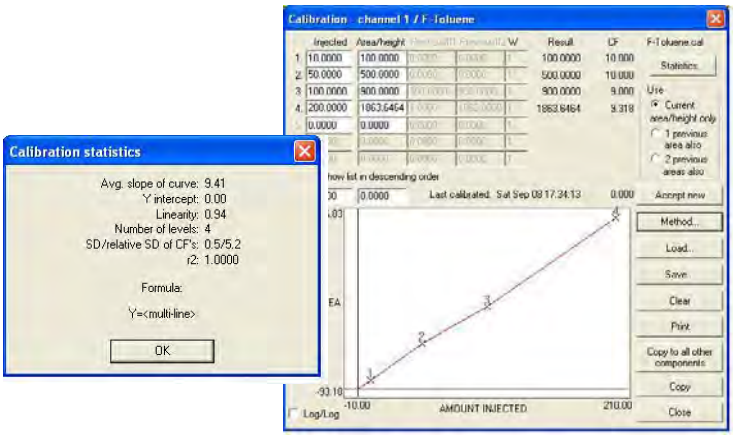
Single line through origin:
The resulting calibration curve is defined as
y=Ax
where: **x is external measure**
y is area
A=(Y/X)/n

Single line:
The resulting calibration curve is defined as
Y=Ax+B
where: x is external measure
y is area
A=((XY*n) – (X*Y)) / D
B=((X*Y2) – (XY*X)) / D
D=((X2*n) – (X*X))

Notes:
This is a least square fit algorithm over the calibration levels. A point at (0,0) is also assumed (by incrementing n) unless there is already a value at x=0, or if [Statistics]R2IncludeZero is set to = in the PEAKWIN.INI file. There must be at least 2 calibration levels. EPA rules allow the use of Single Line Fit provided that the standard deviation of calibration factors is <20%.

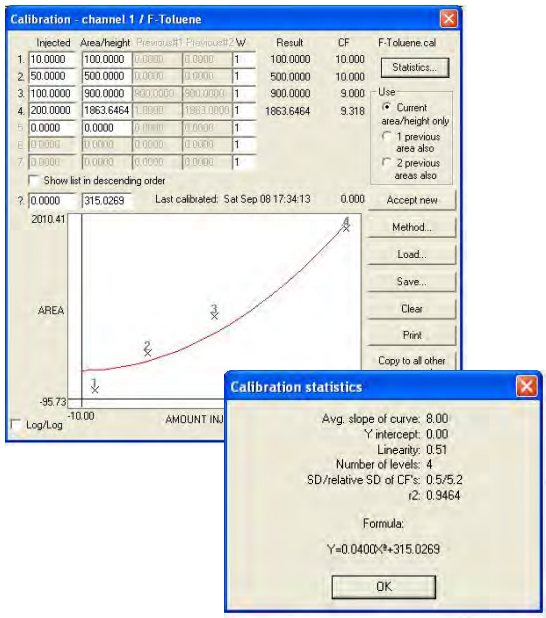


Multiple line segments:
There is no resulting formula here, just interpolation between the levels and the origin. There must be at least one calibration level.

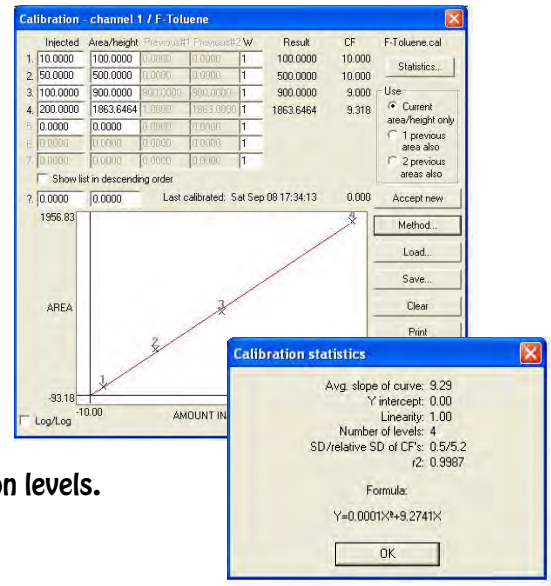


Parabolic:
The resulting calibration curve is defined as
Y=Ax2+B
where: x is external measure
y is area
A=((X2Y*n) - (Y*X2))/D
B=((Y*X4) - (X2Y*X2))/D
D=((X4*n) - (X2*X2))

Notes:
This is a least squares fit algorithm over the calibration levels. A point at (0,0) is also assumed (by incrementing n) unless there is already a value at x=0, or if [Statistics] R2includeZero is



set to 0 in the PEAKWIN.INI file. There must be at least 2 calibration levels (3 if the origin is not assumed).

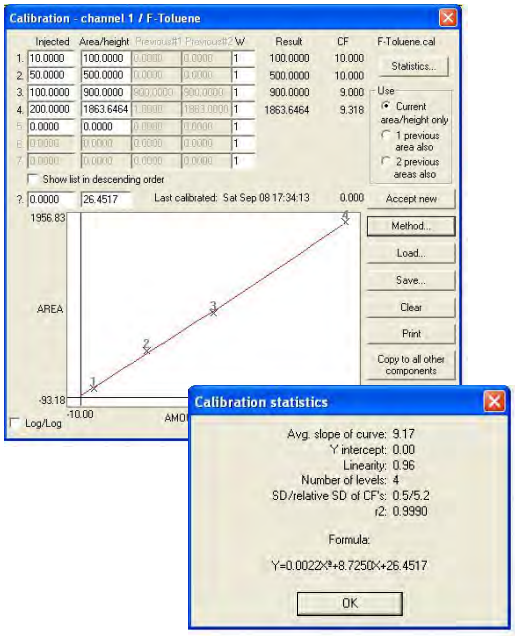


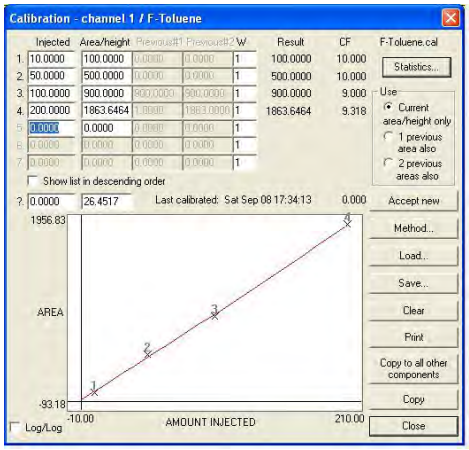
Quadratic through origin:
The resulting calibration curve is defined as
Y=Ax2+Bx
where: x is external measure
y is area
A=((XY*X3)-(X2Y*X3))/D
B=((XY*X4)-(X2Y*X3))/D
D=(X3*X3)-(X4*X2))

Notes:
This is a least squares fit algorithm over the calibration levels. There must be at least 2 calibration levels.

Quadratic:
The resulting calibration curve is defined as
Y=Ax2+Bx+C
where: x is external measure
y is area
A=((XY*X-Y*X2)*(X2*X2-X*X3)-(X2Y*X2-XY*X3)*(X*X-X2*n))/D
B=((XY*X2-Y*X3)*(X2*X3-X*X4)-(X2Y*X3-XY*X4)*(X2*X2-X*X3))/E
C=((XY*X2-Y*X3)*(X3*X3-X2*X4)-(X2Y*X3-X*X4)*(X2*X2-X*X3))/F
D=((X3*X-X2*X2)*(X2*X2-X*X3)-(X4*X2-X3*X3)*(X*X-X2*n))
E=((X2*X2-X*X3)*(X2*X3-X*X4)-(X3*X3-X2*X4)*(X*X2-X3*n))
F=((X*X2-X3*n)*(X3*X3-X2*X4)-(X2*X3-X*X4)*(X2*X2-X*X3))

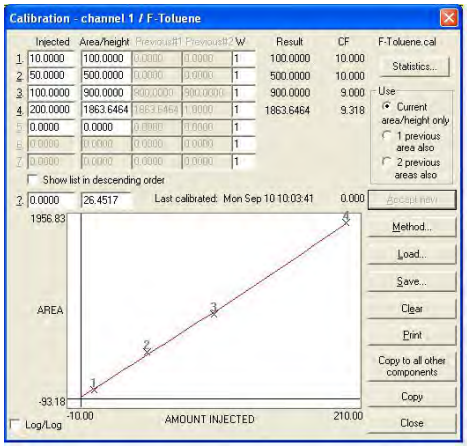
Notes:
This is a least squares fit algorithm over the calibration levels. A point at (0,0) is also assumed (by incrementing n) unless there is already a value at x=0, or if [Statistics] R2includeZero is set to 0 in the PEAKWIN.INI file. There must be at least 2 calibration levels (3 if the origin is not assumed).





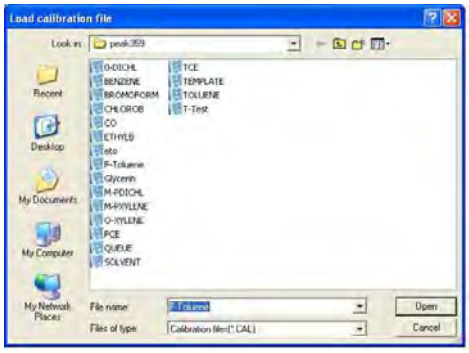
Accept New

If the calibration data is acceptable, click **Accept New** to update the calibration curve data.



Close Button

Automatically saves the new calibration file and closes the Calibration window.

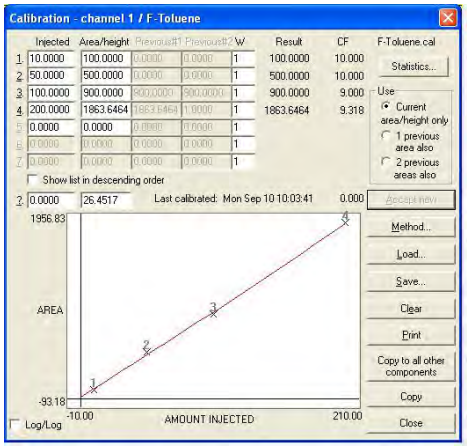


Load

Click on the **Load** button to load an existing calibration file, designated with the **.CAL** file extension.

Save

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



Clear

Clicking on the **Clear** button deletes all calibration data from the calibration window. The calibration file name is also removed.

Print

Clicking on the **Print** button sends the file data and the calibration curve information to the printer.

Channels-Events

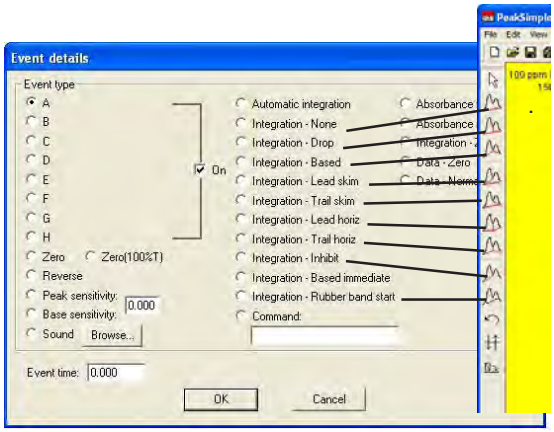
The Events Screen is used to place integration events in a chromatogram for easier data processing. Any of the integration events can saved to the events file where they can be used for subsequent runs.

Change

Click on an existing event to select it. Click on the Change button to change the parameters of the event.

Add

Click on the ADD button to add a new event to the events table. The events details screen will appear to select the new event from. To add an integration event, click on the event and enter the start time at the bottom left of the screen, then click OK.

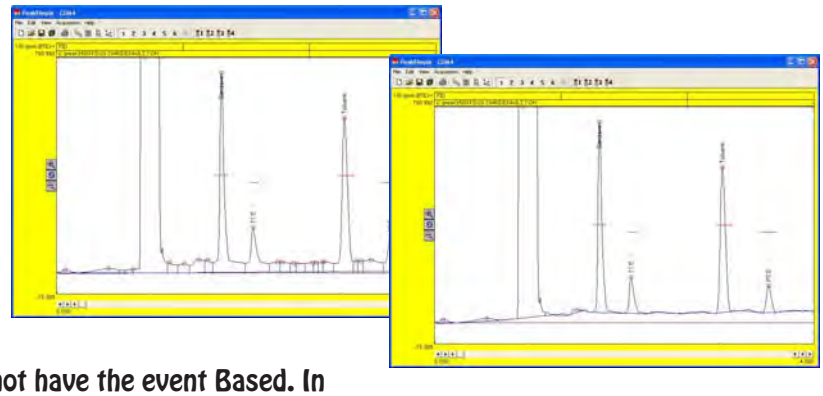


Events A-G are not used in the DPS GC. We use event H to allow PeakSimple to stop the GC program sequence and temperature program.

Using the Zero function zero's the detector signal at the start of the run. This will start the signal at the baseline for better looking chromatograms.

The peak sensitivity features are explained in the Integration section of the manual.

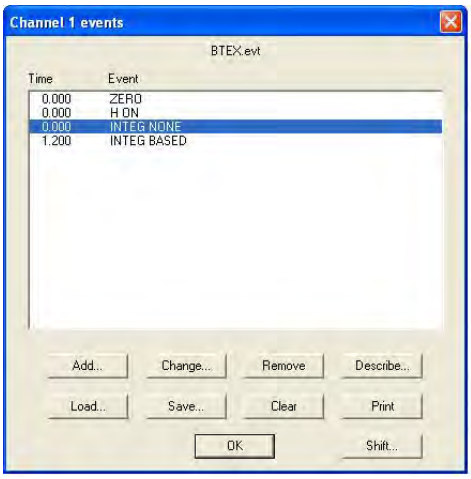
The integration events in the middle of the table follow the same sequence at the Manual Integration events, and are described in detail in that section of the manual. Any of the events can be used multiple times during a run.



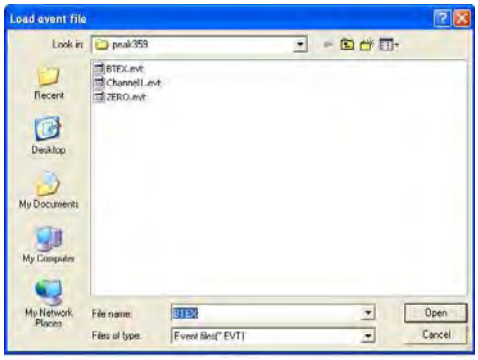
In the example above, the left chromatogram does not have the event Based. In the right chromatogram the event Based is placed at 1.2 min. This event fixes the baseline at the time selected. After this event all of the peaks are quantitated correctly.

The Absorbance buttons on the right side of the screen are for HPLC and not used in DPS GC's.

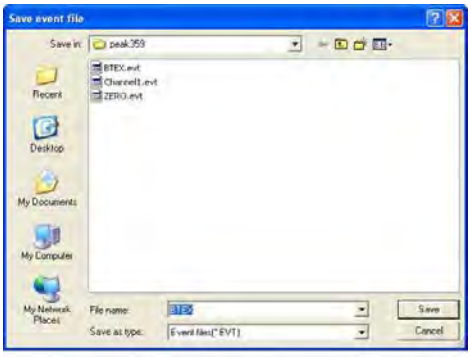
Remove
Click on and event and then the **Remove** button to remove the event from the event table.



Describe
The describe button is for other GC's where they label the events (A-H). The DPS Control Software performs this function in the Systems screen under Configure Names.



Load
Click on the **Load** button to load an existing events file with the **.EVT** file extension.



Save
Click on the **Save** button to save a events file, or to update an existing one.

Clear
Clicking on the **Clear** button deletes all events from the window.

Print
Clicking on the **Print** button sends the events table to the printer.

Channels-Postrun

The Postrun Screen is used to determine all the actions that are to be done in PeakSimple after a chromatogram run. Clicking on the **Postrun** box for channel 1 in the Channel controls window will open up the Channel 1 postrun actions window.

Save file as "X"

The Save file as checkbox, when selected, automatically saves a chromatogram file to disk after a run is completed. The file will be saved under the file name entered in the information field to the right of the checkbox. Please use the default PeakSimple folder for all Saved data!

Auto-increment

When selected, the Auto-increment checkbox will incrementally add a numeric digit to the entered filename after each run. For example, a chromatogram run saved as RUN.CHR would be saved as RUN1.CHR after the second run and RUN2.CHR after the third run.

The **Save results** checkbox, when selected, will save the data in the results screen to disk after a chromatogram run (*Note: This is not the raw data but instead the ASCII results*). The **Add to results log "X"** checkbox adds the results of a run to the results log specified in the information field to its right. It will be saved under the same filename as the raw data but with the extension .RES, for example RUN1.RES.

The **Print results** checkbox will print whatever is specified to be printed in the Print format window, this might include the chromatogram and its results data. The **Update DDE link** checkbox, when selected, will automatically update the Dynamic Data Exchange link once the run is completed.

Execute "X

The Execute information field opens any executable file (.exe, .bat, .bas) after the chromatogram run is completed. *Note: Be sure to include the full filename and path for the executable file.* Control is returned to PeakSimple when the called application closes.

Restart run after "X"

The Restart run after "X" checkbox and information field restarts a chromatogram run after an inputted delay time. The delay time is inputted in minutes and can be repeated as many times as is entered into the times total information field. *Note: If 0 is entered into the times total information field then the run will be restarted after infinite number of times.*

Recalibrate at level "X"

The recalibrate at level "X" checkbox and information field recalibrates all identified peaks at the end of a run at a given level from 1 to 7. This feature is normally implemented as part of an autosampler queue. Detailed instructions are given in the Autosampler queue documentation section.

Smooth first

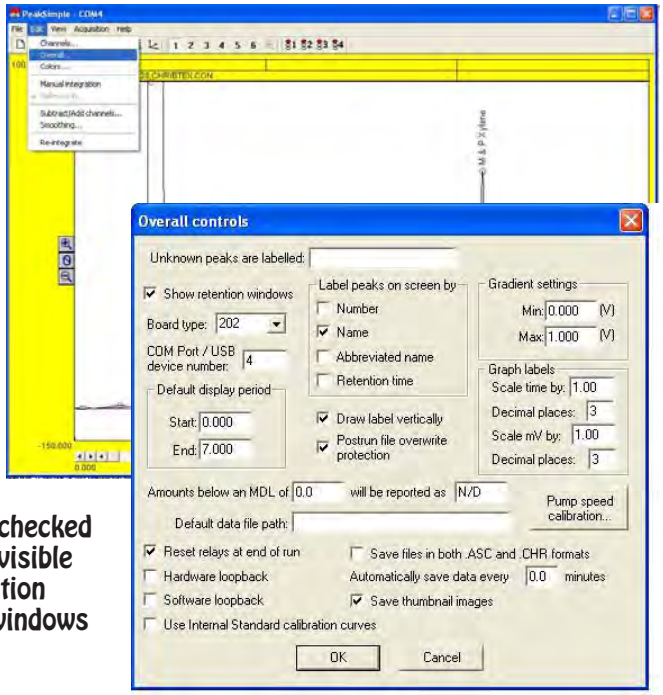
The smooth first checkbox runs the smoothing algorithm as is was last applied to the chromatogram before the final integration is done. If the box is left unchecked no smoothing will be done to the chromatogram run.

Copy data to channel "X"

The Copy data to channel "X" checkbox and information field inputs the chromatogram run into whatever channel is selected in the information field. Only the values 1 to 6 can be inputted into the information field as there are six chromatogram channels in PeakSimple.

Overall Window

The Overall controls window is used to define and control many of the options in PeakSimple. Clicking on **Edit** in the PeakSimple menu bar and then **Overall** from the drop down menu will open up the Overall controls window.



Unknown peaks are labeled "X"

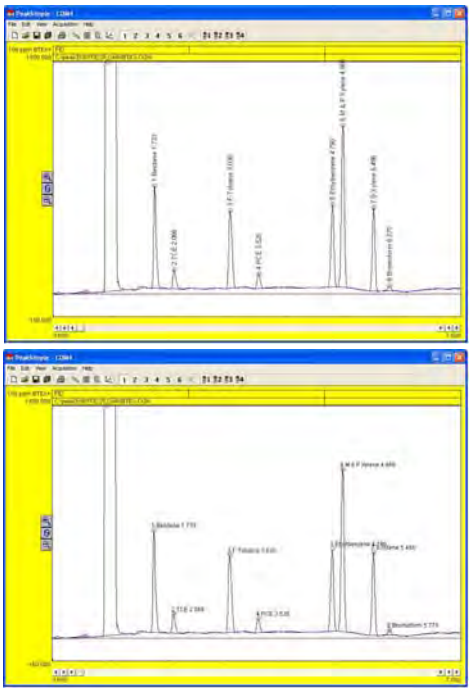
The Unknown peaks are labeled information field, when filled out, labels all unknown peaks the value that is in the information field. If the word "Peak" was entered into the information field then all unknown peaks would be labeled "Peak".

Show retention windows checkbox is checked by default and thus retention windows are visible in PeakSimple; un-checking the Show retention windows checkbox removes the retention windows from sight.

Board Type

By default the board type is set to 202 for all DPS GC's.

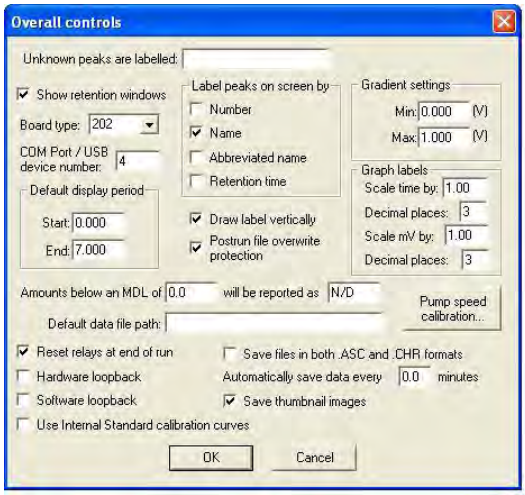
COM Port / USB device number "X" information field specifies the COM port or USB device number that is to be used for the connection between PeakSimple and the hardware. In all DPS GC's where the computer is running in the GC we use COM4. When PeakSimple is running on an external computer we use COM2. We do not use the USB device number.



Label peaks on-screen by

The label peaks on-screen by options box enables a peak to be labeled by as many as four options. The **Number** checkbox labels all peaks with their peak number. The **Name** checkbox labels all peaks with their full name. The **Abbreviated name** checkbox labels all peaks with a shorter, four character abbreviated name while the **Retention time** checkbox labels all peaks with their retention times.

Draw label vertically checkbox specifies whether peaks should be labeled horizontally or vertically on the chromatogram screen. When the box is checked the peak labels will be drawn vertically when it is deselected they will be drawn horizontally.



Default display period

The default display period options box is used to define the default display limits for a PeakSimple chromatogram. The **Start** information field is used to specify the default beginning limits while the **End** field is used to specify the end of the default display limits. The start and end display limits can also be adjusted by the left and right arrows below the chromatogram in the main display window.

Postrun file overwrite protection

Postrun file overwrite protection protects a saved file from being written over when the auto-increment feature is selected in the Postrun window. Instead of writing over a used filename an auto-incremented run will select the next unused number in the sequence to save the file to disk. For example, if file TEST02.CHR already exists on disk PeakSimple will save the file as TEST03.CHR.

Amounts below an MDL of "X" will be reported as "Y"

Peaks with a value below a specified Minimum Detection Level, or MDL will be reported as whatever is specified in the second information field, typically N/D or not detected. The number that is below the MDL will not be reported, only the entry in the second information field will be seen.

Default data file path

Typically all PeakSimple files are saved to the PeakSimple directory but by entering a full directory path into the Default data file path information field another directory can be selected to save files to. *Note: It is recommended that users save all PeakSimple files to the PeakSimple directory. If necessary export files to a different directory after saving them to the PeakSimple directory.*

Reset relays at end of run

The Reset relays at end of run checkbox, when selected, turns off all relays (A-H) at the end of a chromatogram run. If the box is left un-selected the relays will not be shut off after a chromatogram run. In DPS GC's we only use the H relay, all of the other relays are not connected to the GC. The same functions are handled through the **TIMELINE** feature of the DPS GC Control software.

Save files in both .ASC and .CHR formats

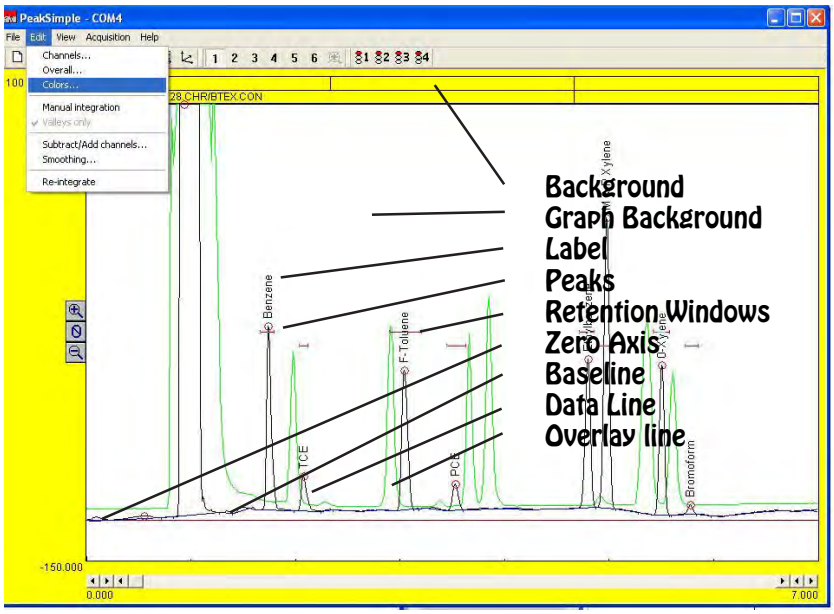
The Save files in both .ASC and .CHR format checkbox, when selected, saves files in the .ASC format (ASCII) and the .CHR format (chromatogram). If the checkbox is not selected files will be saved only in the .CHR format.

Automatically save data every "X" minutes

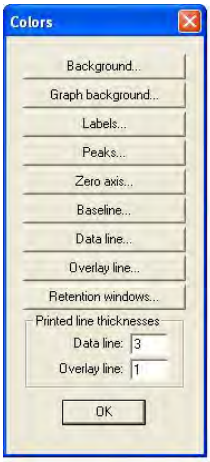
The Automatically save data every "X" minutes checkbox and information field, when selected, saves the data during a chromatogram run at intervals specified by the information in the information field. This feature is useful for runs where power outages are frequent and data can be lost.

Colors

The Colors window determines the color schemes that are to be used throughout PeakSimple. Open the colors window by selecting **Edit** from the PeakSimple menu bar and then **Colors** from the list of options.



Selecting the **Background** button with the mouse cursor opens up the Background color window. The background color can be chosen from a set of 48 colors by selecting a color and then affirming the choice by clicking on the **OK** button.



The Graph background window is opened up by selecting the **Graph background** button in the Colors window. The graph background color is changed by selecting a color and then clicking on the **OK** button to make the color change.

The color of the labels controls the color of the words that belong to the peaks. The color of the labels is changed by selecting the **Labels** button to open up the Labels color window. In the Labels color window select a color and press the **OK** button to make the change to the label color.

The peak color is the color of the circle at the top of each identified peak and is determined by the Peak color window which is opened up by selecting the **Peak** button in the Color window. Select the desired peak color and then click on the **OK** button to close the window and affirm the change.

The color of the zero axis is chosen by clicking on the **Zero axis** button and then selecting a color from the Zero axis color window. Clicking on the **OK** button closes the window and makes the change to the color of the zero axis. Don't set the zero axis color to the same color as the Graph background because they won't be distinguishable from each other.

The baseline is the line that runs along the bottom of the peaks and its color is changed by selecting the **Baseline** button and then choosing a color from the Baseline color window. The change is made once the **OK** button is selected and the window is closed.

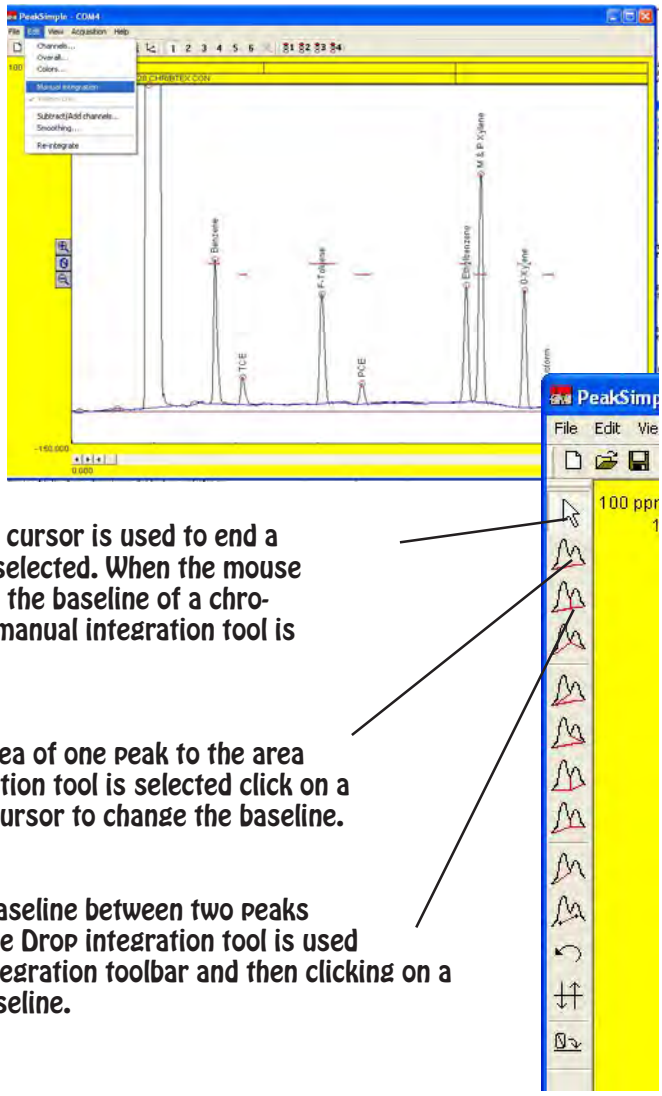
The data line is the signal line that makes up the peaks in PeakSimple and its color is defined by selecting the **Data line** button in the Colors window and then selecting a color from the Data line colors window. Once the desired color is selected apply the color change by clicking on the **OK** button to close the window.

The overlay line is a data line from a chromatogram that has been overlaid on top of an existing chromatogram and its color is changed by selecting the **Overlay line** button in the Colors window and then selecting a color with the mouse cursor in the Overlay line colors window. The color changes are made once the **OK** button is selected and the window closes.

Retention windows are the horizontal bars that appear on-screen and their color can be changed by clicking on the **Retention windows** button in the Colors window and then selecting the desired color in the Retention window colors window. To apply the color changes click on the **OK** button to close the window.

Printed line thickness

The thickness of the Data line and the Overlay line when a chromatogram is printed is determined by the **Data line** information field and the **Overlay line** information field. The thickness of the Data line is determined by the numerical value in the Data line information field, larger numerical values will result in thicker lines.



Manual Integration

The manual integration tools are used to manually draw in a baseline in a PeakSimple chromatogram. The manual integration toolbar is opened up by selecting **Edit** from the PeakSimple menu bar and then clicking on the **Manual integration** option. The manual integration toolbar appears to the right of the PeakSimple toolbar in the upper right hand corner of the screen.

Off Integration Tool

The Off Integration tool or the mouse cursor is used to end a manual integration mode once it has been selected. When the mouse cursor icon is selected no more changes to the baseline of a chromatogram can be performed until another manual integration tool is selected.

None Integration Tool

The None integration tool adds the area of one peak to the area of an adjacent peak. Once the None integration tool is selected click on a valley between two peaks with the mouse cursor to change the baseline.

Drop Integration Tool

The Drop integration tool drops the baseline between two peaks straight down onto an existing baseline. The Drop integration tool is used by selecting the Drop tool in the manual integration toolbar and then clicking on a valley between two peaks to change the baseline.

Based Integration Tool

The Based integration tool raises the baseline to a valley between two specified peaks. To change the baseline select the Based tool and click on a peak with the mouse cursor to raise the baseline up to the valley.

Lead Skim Integration Tool

The Lead skim integration tool skims a peak's area off the leading edge of an adjacent peak. To skim a peak off the leading edge of another peak select the lead skim tool from the manual integration toolbar and then click on the valley between the two specified peaks with the mouse cursor.

Trail Skim Integration Tool

The Trail skim integration tool skims a peak's area off the trailing edge of another, adjacent peak. To skim a peak off the trailing edge of another peak select the Trail skim tool and click on the valley between two peaks with the mouse cursor to make a change.

Lead Horizontal Integration Tool

The Lead horizontal integration tool draws the baseline horizontally for the leading peak while the trailing peak's baseline stretches from the horizontal line to the next valley. The Lead horizontal tool is selected in the manual integration toolbar and once a valley is selected the change to the baseline is made.

Trail Horizontal Integration Tool

The Trail horizontal integration tool draws a baseline horizontally for the trailing peak while the leading peak's baseline stretches from the horizontal line to the previous valley in the chromatogram. The Trail horizontal tool is used by selecting the Trail horizontal tool in the manual integration toolbar and then clicking on a valley with the mouse cursor to make the change.

Inhibit integration Tool

The Inhibit integration tool ends a baseline after a valley thereby stopping the peak's area from being counted along with the rest of the chromatogram. To use the Inhibit tool select the tool in the manual integration toolbar and then click on the valley between two peaks to end the baseline.

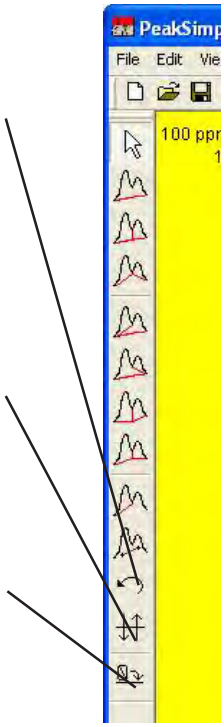
Rubber Band Integration Tool

The Rubber band integration tool is used to manually draw the baseline in a chromatogram. The Rubber band tool is selected in the manual integration toolbar and is clicked an dragged on the chromatogram to draw the baseline.

Undo Integration Tool

The Undo integration tool removes all changes done to the baseline of a chromatogram with the manual integration tools. To use the Undo tool click on the tool in the manual integration toolbar and all changes will be undone.

Note: Changes made to a chromatogram with the Reverse and Zero integration tools cannot be undone with the Undo tool.



Reverse Integration Tool

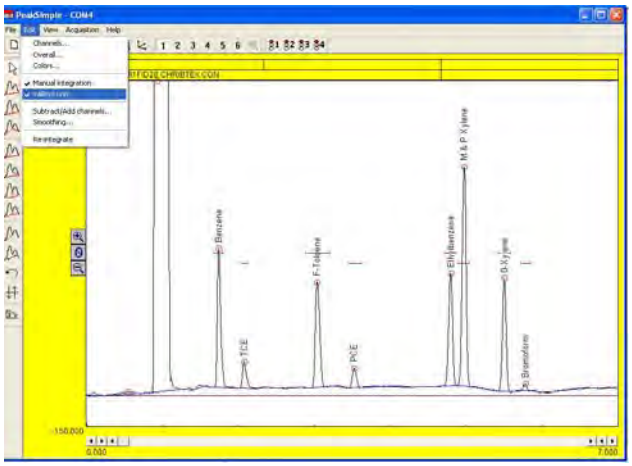
The Reverse integration tool inverts a selected peak or a selected group of peaks in a chromatogram. A peak is inverted by selecting the Reverse tool in the manual integration toolbar and then clicking and dragging the mouse cursor over the peak.

Zero Integration Tool

The Zero integration tool sets the value of the data line at zero starting at a selected point. To zero the data line at a given point select the Zero tool from the manual integration toolbar and click on the data line with the mouse cursor.

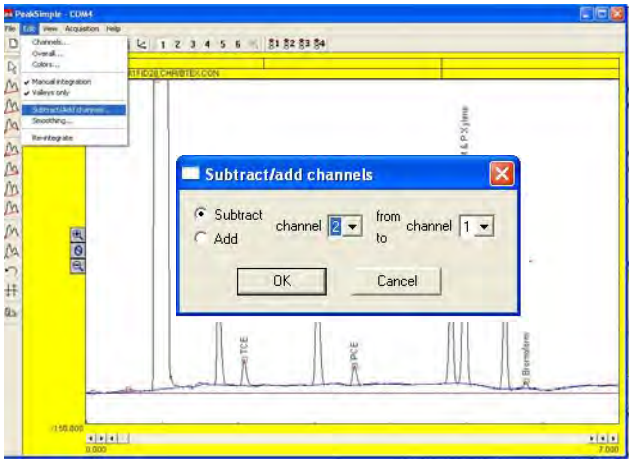
Valleys Only Option

The Valleys only option is available only when the Manual integration toolbar is open in PeakSimple. The Valleys only option can be selected by opening up the Manual integration toolbar in the Edit menu and then selecting the Valleys only option immediately below Manual integration in the drop down menu. When the Valleys only option is selected all changes made to the baseline of a chromatogram will snap only to the valleys of the chromatogram. When the Valleys only option is turned off changes made to the baseline of a chromatogram will go to wherever the mouse cursor was clicked.



Subtract/Add Channels Menu

The Subtract/Add channels menu removes or adds the analog data signal from/to one channel in PeakSimple from/to another channel. The Subtract/Add channels menu is opened by selecting the Edit menu and then by clicking on Subtract/Add channel in the drop down menu.



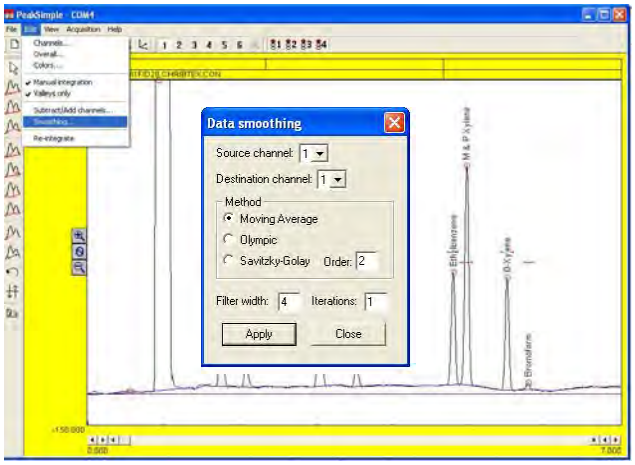
Subtracting a Channel

To subtract one channel from another channel click on the Subtract radio button with the mouse cursor and select the channel that is to be taken away in the first dialogue box. In the second dialogue box select the channel that is to have the first selection taken away from. Click on OK with the mouse cursor to effect the changes.

Adding a Channel

To add one channel to another channel select the Add radio button in the Subtract/Add channels menu. Select the channel that is to be added by selecting a number in the first dialogue box and then choose the channel that it is to be added to by selecting a number in the second dialogue box. All changes are made once the OK button is selected.

Smoothing Window



The Data smoothing window determines all the smoothing options that are to be performed on a data line. The Data smoothing window is opened by selecting Edit from the PeakSimple menu bar and then selecting Smoothing from the list of options.

The **Source channel** dialogue box specifies which channel the data line that is to be smoothed is in. The **Destination channel** is the channel that the smoothed data line from the source channel will be displayed in.

Method

The method of smoothing is determined by the smoothing algorithm selected in the Method box. The **Moving Average** algorithm sets each sample to the average of the samples around it including itself. The number of samples taken into account depends on the Filter width. The **Olympic** algorithm is similar to the Moving Average but the highest and the lowest values in the set of samples are discarded before the average is taken. The **Savitsky-Golay** algorithm is similar to the Moving Average but each of the samples is weighted according to a set of weighting factors. Increasing the number of in the **Order** dialogue box gives more weight to the central samples when using the Savitsky-Golay method.

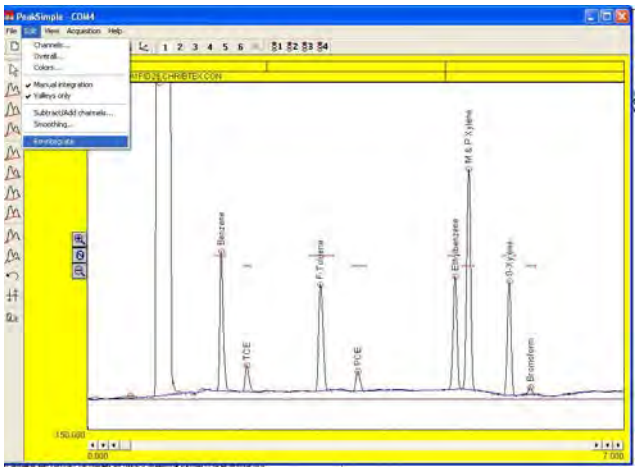
Filter Width The Filter width dialogue box controls the number of samples that are to be taken into account when using the Moving Average smoothing method. A filter width of 2 means that 2+1+2 samples are taken while a filter width of 5 means that 5+1+5 samples are taken.

Iterations

The Iteration dialogue box controls the number of items a smoothing method is to be applied to a chromatogram peak. Every iteration smooths the data line more than the previous iteration eventually making the data line flat.

The Re-Integration Option

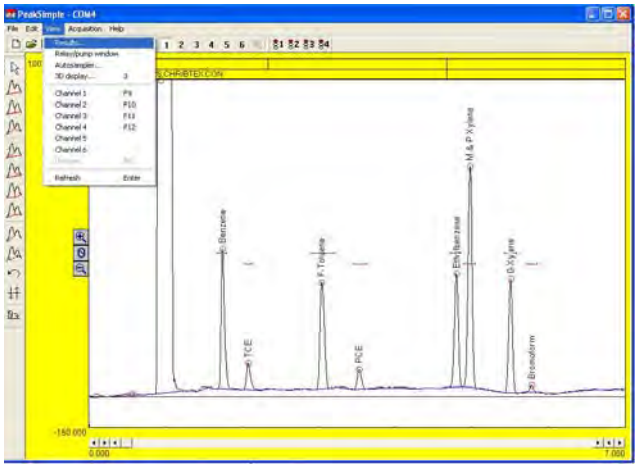
The Re-Integration option is used to fully re-integrate a baseline in PeakSimple. When changes are made to a baseline often a partial integration will occur, selecting Re-integrate will perform a full integration on the baseline. The Re-integrate option can be selected by clicking on Edit in the PeakSimple menu bar and then Re-integrate from the list of options.



View Pull-Down Menu

EDIT-View-Results Window

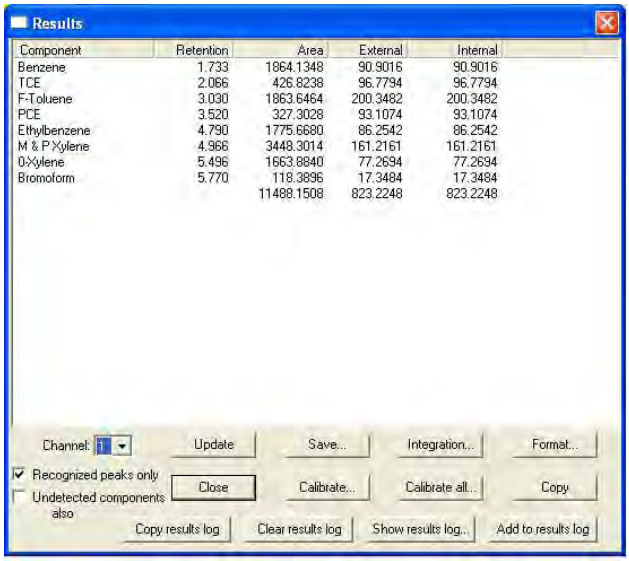
The Results window displays the results of the chromatogram runs performed in PeakSimple. The Results window is opened by clicking on View in the PeakSimple menu bar and then selecting Results from the list of options.



The **Channel** option scroll bar specifies which of the six channels the results data should be displayed for. When the **Recognized peaks only** checkbox is selected only the results for named peaks will be displayed. The **Undetected components also** checkbox displays the results for the undetected components as well as the detected components in the chromatogram run when the option is selected.

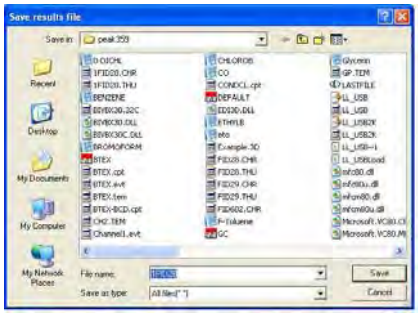
Update

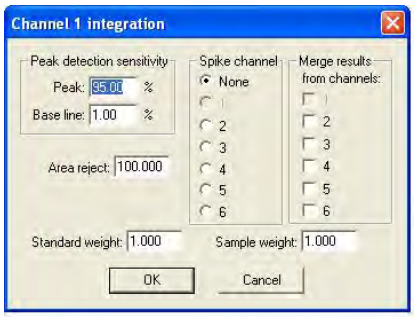
The Update button in the Results window updates the DDE link between the Results data and the DDE host program (typically Excel).



Save

Selecting the Save button in the results window opens up the Save results file window. In the Save results file window the results file is saved with a .res extension. The file is an ASCII file and not the raw chromatogram data.



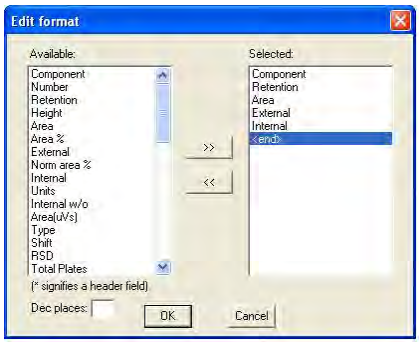


Integration

As a convenience the integration button in the results window opens upon the same integration window that can be accessed in the Channels window. For more information on the integration window consult the Channels-Integration portion of this manual.

Format

Selecting the Format button in the Results window opens up the Edit format window. The Edit format window allows the user to specify the information that is to be included in the Results table. The **Available** options box in the Edit format window displays all the available options that can be included in the results but that aren't selected. An option is added to the **Selected** options box by highlighting the item in the Available box and clicking on the right facing arrow button. To deselect an option from the Selected box highlight the item and click on the left facing arrow button. The **Dec. places** dialogue box specifies how many decimal places a highlighted unit will display in the Results table.

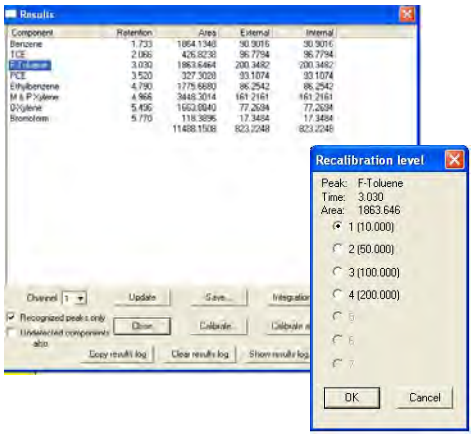


Close

The Close button exits the Results window and returns the user to the main screen.

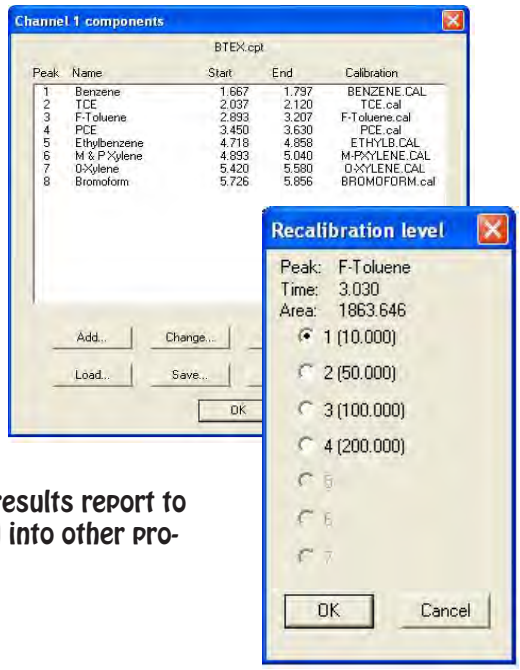
Calibrate

The Calibrate button recalibrates a recognized peak in the Results table. Highlighting a peak name and selecting the Calibrate button opens up the Recalibration Level window. The window specifies which peak level should be calibrated. Following the Recalibration level window is the Calibration window which is discussed at further length in the Calibration section of this document.



Calibrate All

The Calibrate all button recalibrates all the recognized peaks at once. The Calibrate all button calibrates all peaks with existing calibration curves on a particular calibration level. If named peaks are in the results table without calibration curves an error message (NOT ENOUGH DATA POINTS), will be displayed. Check the Components table to make sure that all compounds have Calibration curves associated with them.



Copy

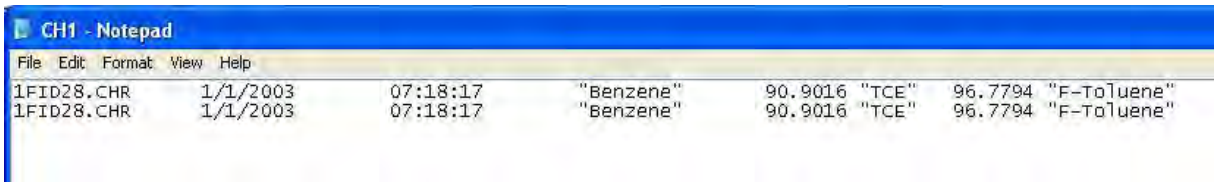
The Copy button in the results window copies the results report to the Clipboard. Once the report is copied it can be pasted into other programs i.e. Excel.

Copy Results Log

The Copy results log button copies the .log file for the results to the Clipboard. This log file can be pasted into any Windows program. A certain number of lines in the results log will always be copied, by default the number is 20. If more than 20 lines are needed for an application the user must modify the peakwin.ini file located in the Windows folder. The default entry in the files is (SpareLines=20), delete the number 20 and insert the number of lines that are needed (up to a maximum of 100).

Clear results Log

Clicking on the Clear results log button erases the results log file.



Show Results Log

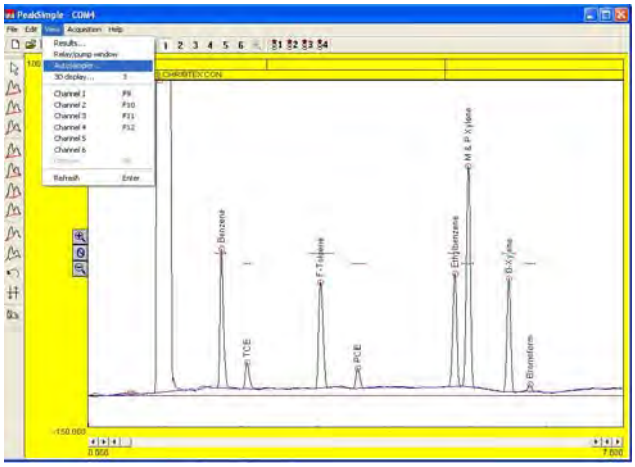
The Show results log button opens up the Windows Notepad to view the results log.

Add to Results Log

To add the current report to the results log click the Add to results log button. The report can automatically be added to the results log at the end of each chromatogram run by checking the Add to results log checkbox in the Postrun window.

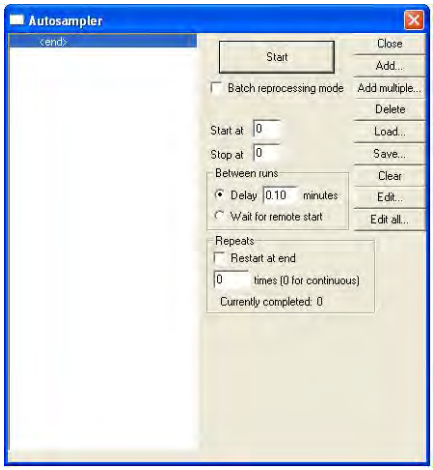
View Autosampler Window

The Autosampler window allows a list of control files to be run automatically. Control files are the master files which specify all parameters including temperature programming, component, and event files. These control files run tasks in PeakSimple. To open up the Autosampler window click on the View menu in the menu bar and then select Autosampler from the available options.



Start/Stop

The Start button, when pressed, begins the operation of the autosampler queue or reprocessing queue. A queue must be created or loaded before the control files can run. Once the autosampler is in operation the Start button changes into the Stop button. The Stop button ceases the autosampler operations that were previously running.



Batch Reprocessing Mode

To select Batch reprocessing mode click on the check box to the options left. While using the Batch reprocessing mode the user loads a list of previously stored chromatogram files in the list box of the left and then selects a control file which reprocesses the data files. When the operation begins PeakSimple will load each data file in the list into channel 1, perform the specified functions, and then increment to the next data file in the list.

Start at dialogue box specifies which control file number to begin operation first. If no number is entered the autosampler will begin at the first control file.

Stop at dialogue box specifies the last control file to be run before operations of the autosampler cease. If no number is entered in the dialogue box the autosampler will end after the last control file in the list is run.

Delay "x" minutes radio button, when selected, specifies how many minutes PeakSimple will wait before running the next control file in the list box.

Wait for remote start radio button, when selected, instructs the autosampler to wait for a remote start signal before advancing to the next control file.

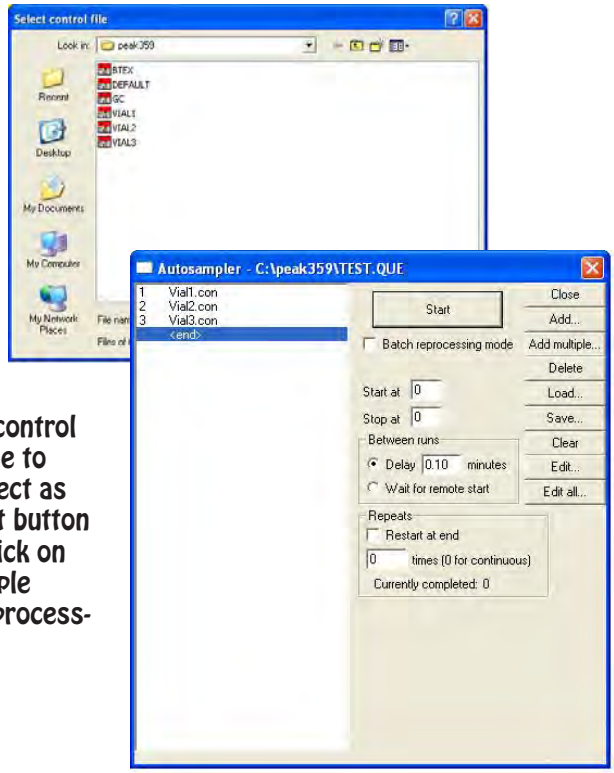
Restart at end checkbox restarts the queue after getting to the end of the control files in the list box. In the **"x" times** information field the user enters the number of times the control files in the list box should be cycled if the Restart at end checkbox is selected. If the value 0 is selected, the queue will be cycled continuously.

Close

The Close button closes the Autosampler window when it is selected.

Add

Select the Add button to add a control file to the queue. Selecting the button opens the Select control file window where the file can be loaded into the list box. Each control file in the queue must have a different name even though almost identical actions are performed.



Add Multiple/Batch Reprocessing

The Add multiple button allows the user to load multiple data files into the list box. Click on the button to open up the Select control file window and then click on a control file name to open up the Select data filenames window. Select as many data files as needed by pressing the shift button and clicking with the mouse cursor and then click on OK to load them into the queue. The Add multiple button is only useful for use with the Batch reprocessing mode.

Delete

After highlighting a control file in the list box to the left select the Delete button to remove that control file from the queue.

Load

Select the Load button to open up a previously saved queue file. Clicking on the Load button opens up the Load autosampler queue window where the queue file can be selected and loaded.\

Save

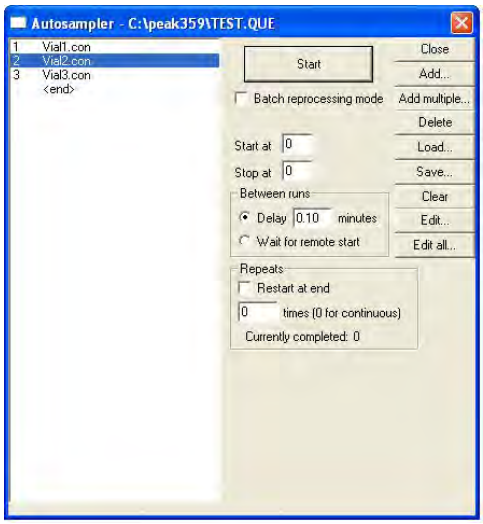
Selecting the Save button opens up the Save autosampler queue window. Save the queue in the file box by naming the file and selecting Save. It is recommended that all files are saved to the PeakSimple directory.

Clear

The Clear button erases the entire queue.

Edit

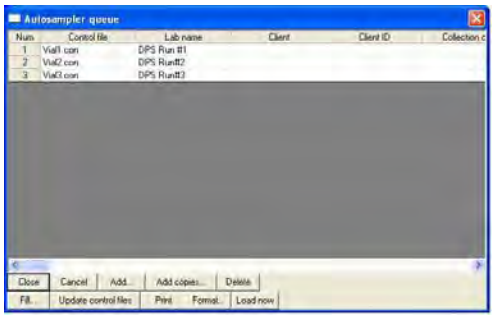
After highlighting a control file select the Edit button to modify that control file. Selecting the Edit button loads the control file on the PeakSimple main screen. To make any changes click on the main screen, do all modifications, and then select Save all from the PeakSimple file menu



Edit All

To edit all the control files in the queue at once click on the Edit button to open up the Autosampler queue spreadsheet. Many of the commonly adjusted control file parameters are displayed in the spreadsheet enabling the user to input changes to the queue. Not all control file parameters can be modified by using Edit all (only parameters that are selected in Format) and so must be done individually with the Edit function.

Autosampler Queue Window



Close

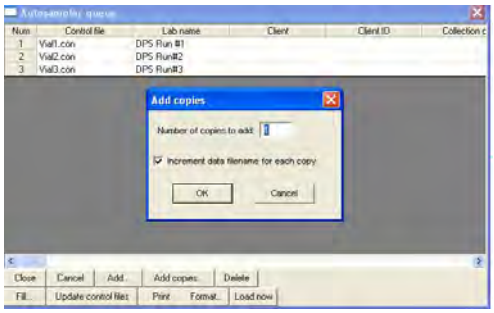
The Close button exits the window after prompting the user to save the spreadsheet.

Cancel

The Cancel button exits the spreadsheet window without prompting the user to save.

Add

Selecting the Add button opens up the Select control file window where an existing control file can be added to the queue.



Add Copies

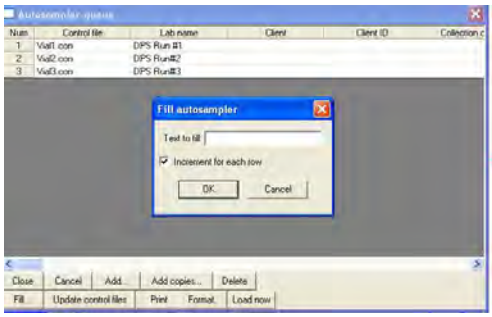
After highlighting a control file in the spreadsheet select the Add copies button to add copies of the file to the list. Once the Add copies window pops up input the number or copies to be made in the dialogue box and specify whether the file names should be incremented. The Add copies button is useful for creating a queue from scratch with a single control file.

Delete

The Delete button deletes a highlighted control file off the list. If no file is highlighted then the last file bill be deleted from the queue.

Fill

The Fill button fills a spreadsheet column, row, or cell with selected text. Once the desired cells are highlighted clicking the Fill button opens up the Fill autosampler options box. Input the text to fill in the information field and specify whether the text should be incremented for each row.



Update Control Files

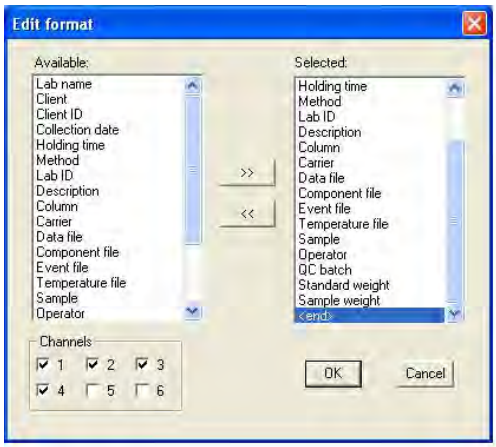
Selecting the Update control files button saves all changes to the control files in the list.

Print

The Print button prints the queue spreadsheet.

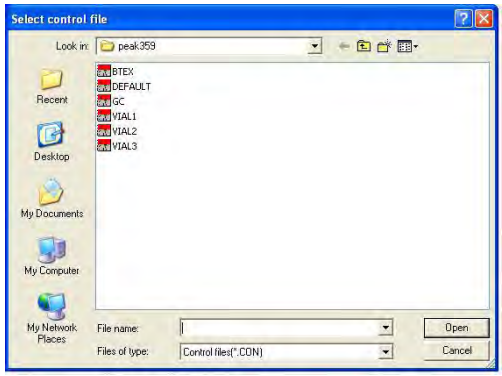
Format

To change the format of the queue spreadsheet and open the Edit format window select the Format button. In the Edit format window a format type can be added by selecting it in the Available window and then hitting the right facing arrow button. To remove a format type from being displayed in the spreadsheet highlight the format type in the Selected box and click on the left facing arrow.

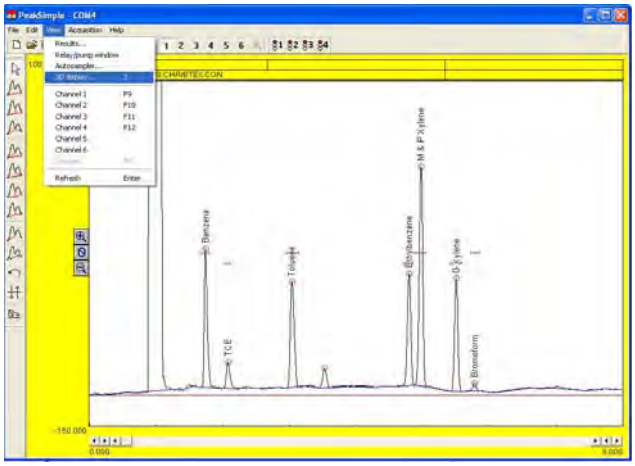


Load Now

After highlighting a control file select the Load now button to load that control file to the main PeakSimple screen. Click on the screen and make any changes to the control file and then select Save all to save the changes.



3D Display Window



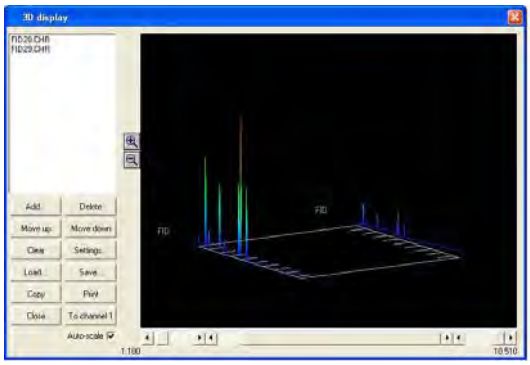
To view the 3D Display, select 3D in the View window. The 3D display allows you to load multiple chromatograms and view the in 3D. The display can be rotated to view trends over time. No quantitative data can be generated through the 3D display, but it is a valuable tool for viewing trends.

Add

To Add chromatograms to the display, select the individual chromatograms.

Delete

The Delete button will Delete the highlighted chromatogram.



Rotate

By holding down the right mouse button you can rotate the 3D display 360 degrees to view trends.

Move Up

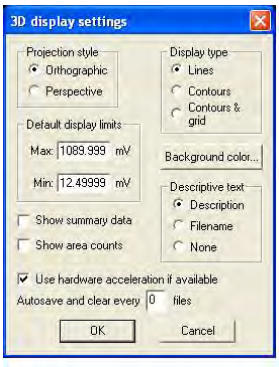
Moves the selected chromatogram up one position.

Move Down

Moves the selected chromatogram down one position.

Clear

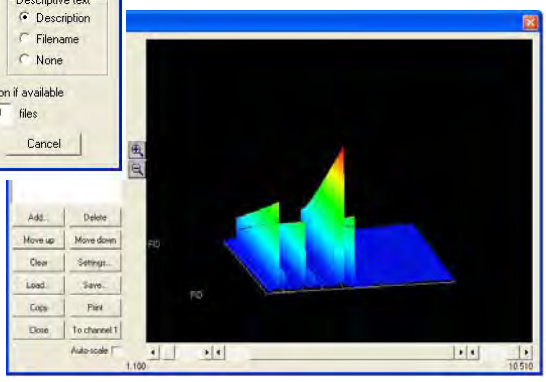
The Clear button clears all data from the 3D display.



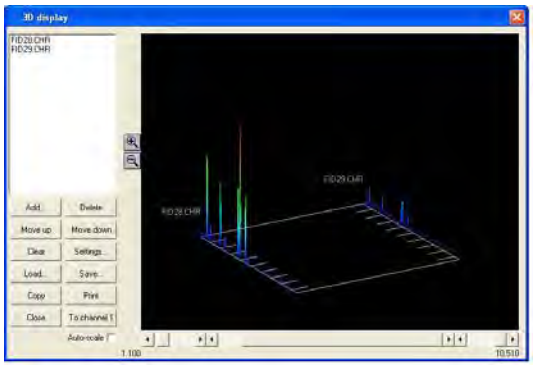
Settings

The Settings screen allows you to change many variables in the 3D display. The Display type, Colors, data Description, and default limits can be easily be changed.

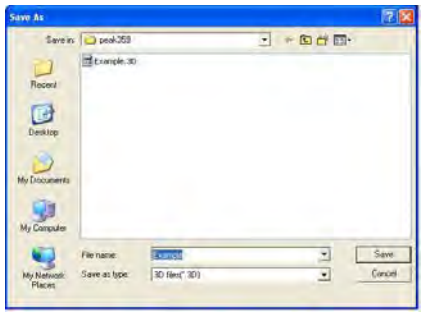
An example of contours and grid is shown to the right.



Load
Loads a chromatogram into the 3D display.



Save
Saves the contents of the current 3D display. The display can be viewed again using the Load command.

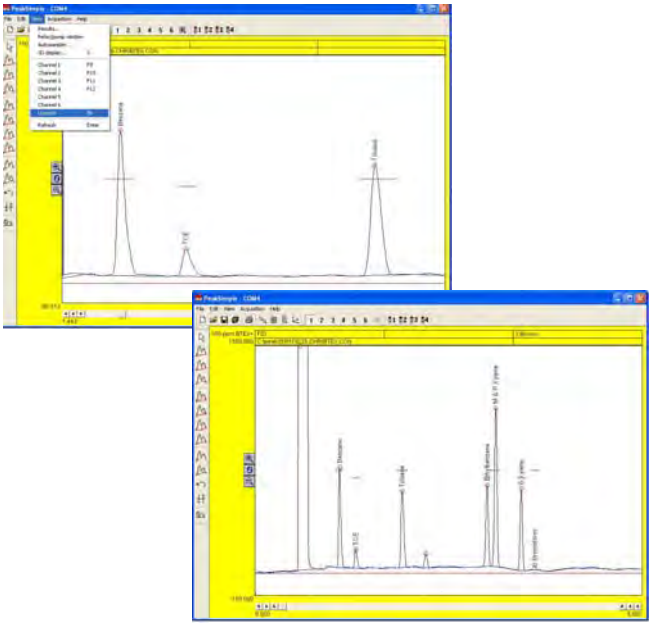


Copy
Copies the current display to the the Windows clipboard.

Print
Prints the display to the default printer.

Close
Closes the 3D display.

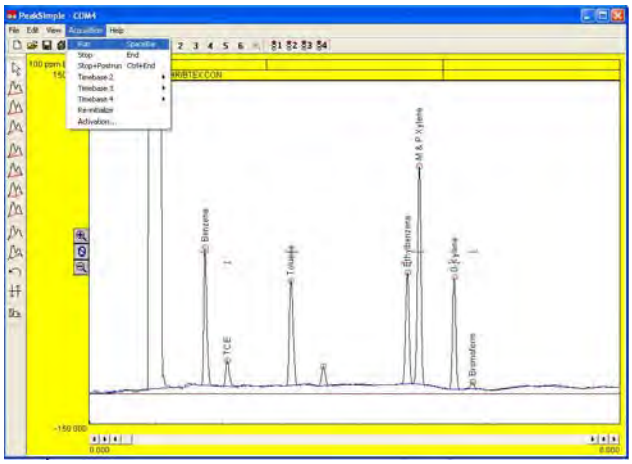
View Unzoom
To unzoom from a close up view of a chromatogram select the Unzoom tool from the View menu or hit F6. Peak-Simple will zoom out to the first level with the original display units of the chromatogram when the Unzoom tool is used. The Unzoom button in the Peak-Simple toolbar can also be used to unzoom a chromatogram or F6 on the keyboard.



Refresh

The Refresh tool in the View menu redraws the chromatogram screen to fix any glitches or resolve an error. Pressing Enter on the keyboard also refreshes the screen.

Acquisition Pull-Down Menu



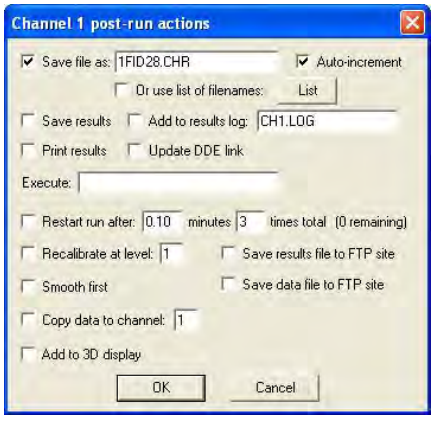
The Acquisition menu contains the commands to run a chromatogram run when hardware is connected to the PeakSimple data system. All Acquisition menu commands have corresponding keyboard hot-keys for convenience.

Run

The Run command begins a chromatogram run on the main trigger group when hardware is connected to the data system. The error message "No active channels in group" appears when no hardware is available to make a chromatogram run. The spacebar can be used to start a run.

Stop

The Stop command is used to end a chromatogram run once it has been started. Using the Stop command ends the chromatogram run without running any of the Postrun operations. The End button can also stop a chromatogram run.

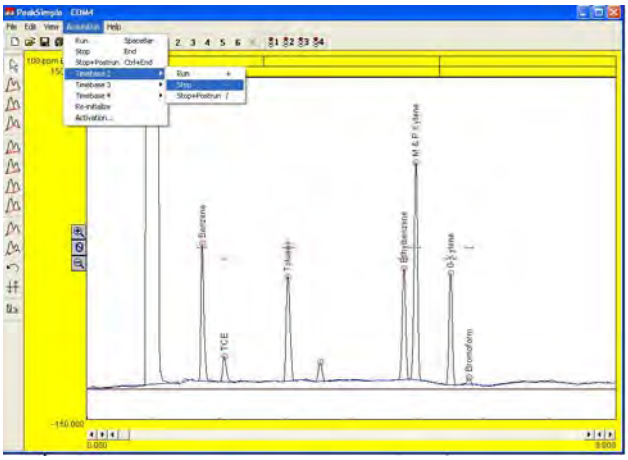


Stop + Postrun

The Stop+Postrun command ends a chromatogram run and executes the operations specified in the Postrun section. Holding the Control button and pressing End on the keyboard is the same as the Stop+Postrun command.

Timebase

The Timebase function in PeakSimple allows you to remotely trigger up to 4 chromatographs. We do not use this function in DPS GC's. All channels on a single GC start with the **RUN**, or **SPACEBAR** buttons.



Re-initialize

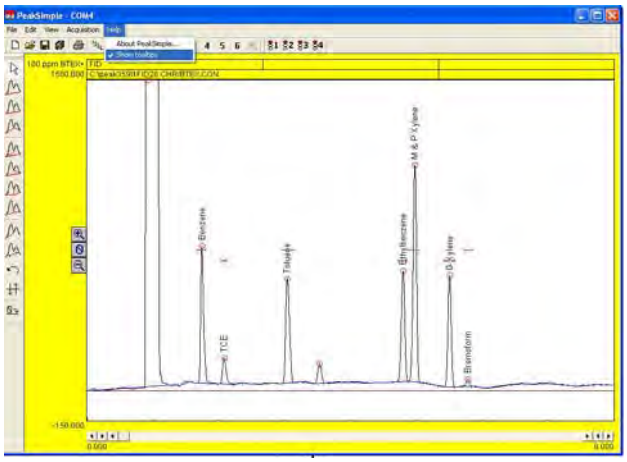
The Re-initialize command reestablishes the connection between the hardware and the PeakSimple data system. A connection between hardware and the data system has to exist for re-initialization to occur.

Activation

The copy of PeakSimple is already activated when it arrives in the GC. A Serial Number accompanies the paperwork with the GC. Activation is for customers that have downloaded PeakSimple and want to demo the software before purchasing. Once they have purchased it, the manufacturer supplies an activation number. There is no need to look for, or enter an activation number.

HELP Pull-Down Menu

The **EDIT** pull-down menu allows you to modify most of the operating parameters.



About PeakSimple

To view program information about PeakSimple click on the About PeakSimple option in the Help menu. The PeakSimple window will pop up and display the information.

Show Tooltips

The Show tooltips option in the Help menu toggles the PeakSimple tooltips off or on. When Show tooltips is checked a helpful text tip will appear when the mouse cursor is held over a tool or button in PeakSimple. The tooltips provide relevant information to the operation and use of the PeakSimple data system. Most of this manual is contained on the tool tips, which is a convenient way of learning the software.