# Instructions for Using the PeakSimple Chromatography Data System
Revised 10/7/09 for PeakSimple Version 3.78

The PeakSimple Chromatography System is a data acquisition hardware and software package designed to collect and analyze data from separations experiments. While the package has some functions that allow limited hardware control, this guide will only focus on data acquisition. With appropriate knowledge of the instrument, PeakSimple can be coupled with both GC and LC systems easily. Refer to the PeakSimple manual for information on making physical connections to the hardware.

1. Locate the power button on the back of the PeakSimple interface box and turn it on. The red "POWER" light on the front of the box should light.

2. Locate the PeakSimple software on the computer. Look for an icon labeled "Peak378" or "PeakSimple". It is likely that an icon exists on the desktop, if not, use Windows Explorer to find the folder C:\peak378" and click on the "peak378.exe" file.

3. The program will take a few moments to begin as it locates and initializes the hardware. If an error message appears, click "OK" to clear the message and in the **Edit** menu, select **Overall…** The window below should appear. This window specifies several settings for communication between the data system and computer.
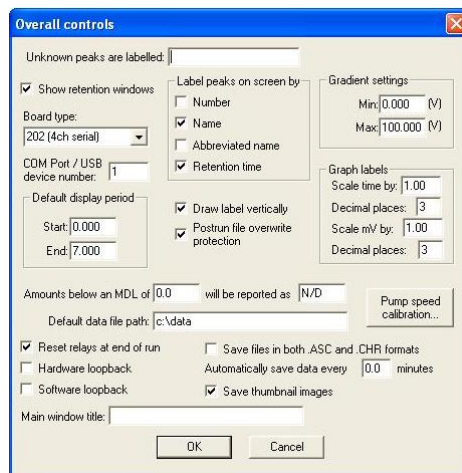

For communication with the data system, the **Board Type** must be set to "202 (4ch serial)" and the **COM Port/USB device number** set to "1". From this window you can also set the default folder for data storage. In the window above, it is set to the "c:\data" folder. The default settings are typically fine for the rest of the window. Once all settings are correct, click **OK** to apply them.

<u>**Software Setup:**</u>
Before collecting data, you must let the system know where it should look for the data, how you would like it collected, and how the data should be treated after collection.

1. In the **Edit** menu, select **Channels…**. The window below should appear. This window allows access to a host of parameters related to data collection and handling.
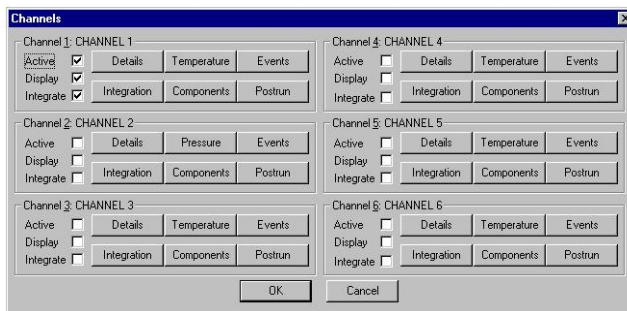

2. Using PeakSimple, it is possible to collect data in each of several channels. For example, you might wish to collect absorbance data from an HPLC detector on Channel 1 and pressure data from the HPLC pump on Channel 2. In order to accomplish this, parameters for each Channel must be set. For most situations, the key aspects of this window are the "**Details**" and "**Postrun**" buttons for each channel.

3. The "**Details**" button allows you to control how data is collected on a given channel. Clicking on the button brings up the window below.
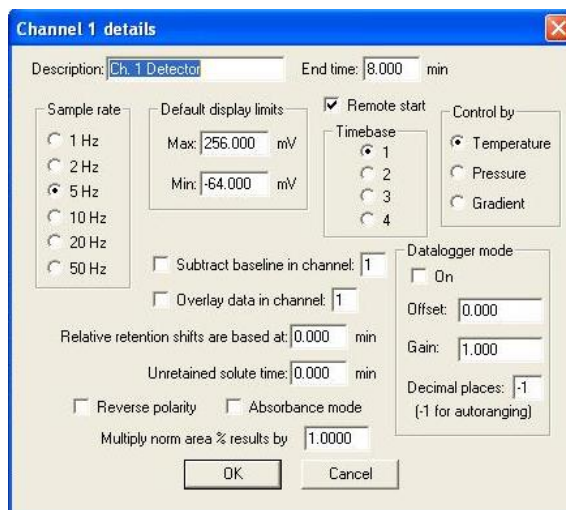
In this window, enter an **End Time** that exceeds the expected duration of your separation. Select a **Sample rate** that is appropriate for your separation as well. A good rule of thumb is to use a sampling rate that gives you at least 20 data points across a peak. Therefore if a peak takes 10 seconds to elute, a minimum sampling rate of 2 Hz is suggested. Extremely large sampling rates may result in excessive noise and unnecessarily large data files. If you would like PeakSimple to initiate data collection automatically when an injection is made (and if the hardware is set up to do so), be sure that the **Remote start** box is checked. Once you have finished, click **OK** to return to the **Channels…** window. Repeat this for each channel for which you would like to collect data.

4. From the **Channels…** window, click on the **Postrun** button to bring up the window below.
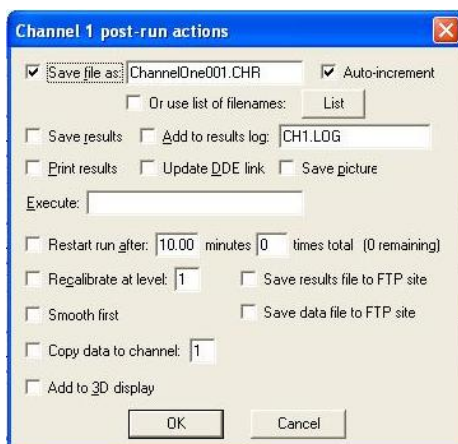
From this window, you can control how the data is stored after your run. Since data files are relatively small and storage space fairly cheap, it is wise to have the program automatically save your data after each run. Check the "**Save file as:**" box and enter a filename in the field to accomplish this. If you also check the "**Auto-increment**" box, PeakSimple will save each file under a new name created by incrementing a number at the end of the filename. This is a very good idea, otherwise data is likely to be overwritten.

Data Collection:
Once collection parameters have been set, data collection is a breeze. In most cases, PeakSimple will be configured to initiate data collection when a sample is injected. Data collection can also be initiated through the **Acquisition** menu or by pressing the spacebar. Collection will continue for the duration specified in the **Details** section for a particular channel. Data collection can also be stopped through the **Acquisition** menu or by pressing the *End* key.

During data collection, you can zoom in or out of the chromatogram using the buttons on the left of the plot. Pressing the zero button will adjust the data so that the current value is reassigned to zero. The slider on the bottom of the window can be used to adjust the x-axis range.

Data Analysis:
For each component in a separation, two pieces of data are typically of interest; the retention time for the peak and the peak area. Each of these parameters is readily determined using PeakSimple.

1. After completion of a run, PeakSimple will attempt to identify peaks using the parameters set up in the **Integration** tab of the **Channels…** window. Peaks that have been identified will bear a red circle at the peak. To determine the area under the peak right-click on the circle and select "**Add Component**" from the menu that pops up. A bar will be placed across the peak and the peak will be labeled with its retention time. Repeat this operation for additional peaks. To view a table of peak areas and retention times, click on the "**Results**" icon at the top of the screen or select **Results** from the **View** drop-down menu.

2. You may also manually enter a peak by right clicking on the chromatogram, selecting "Add Component", and manually positioning the bar over the peak of interest. Clicking and dragging on either end of the bar will allow you to adjust the size of the bar. Open the **Results** window to see the outcome of this operation.