

PEAKSIMPLE SOFTWARE

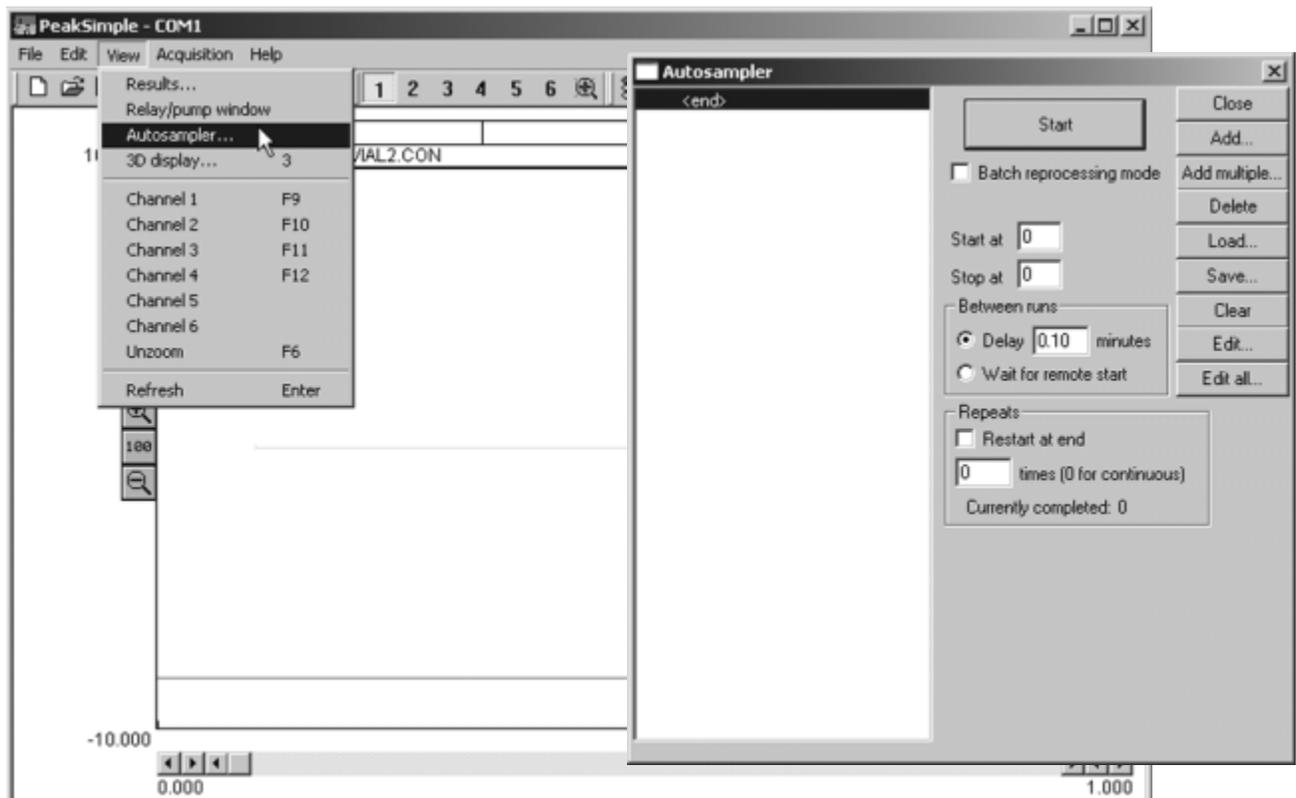
Autosampler Queue

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

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

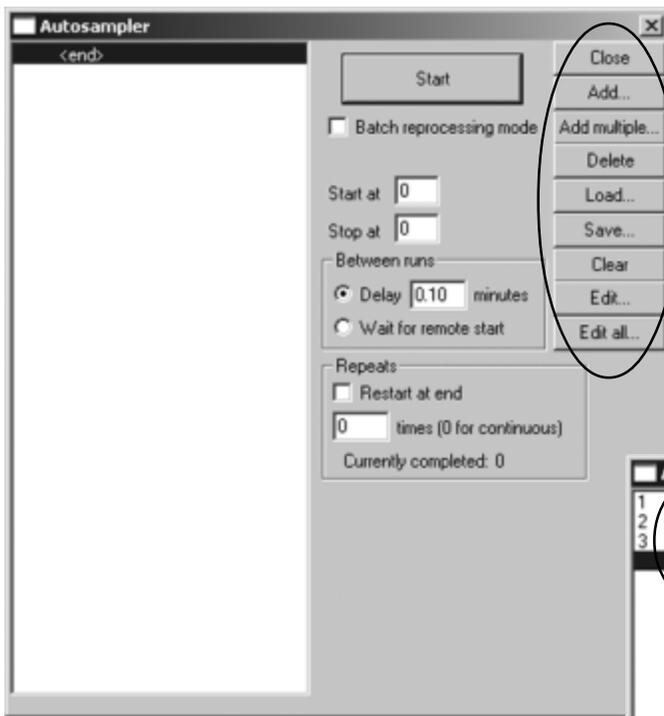
Each control file in the list must have a unique name, even if it is identical to others. It is helpful to include a number in the name of each control file that corresponds with its place in the list; for example: Vial01.con, Vial02.con, Vial03.con, etc. The control file(s) you wish to use in the Autosampler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

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



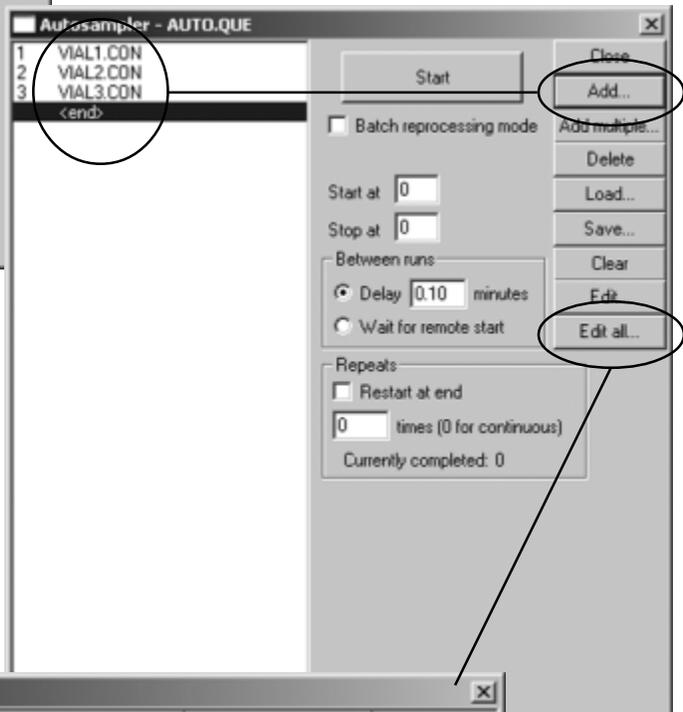
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Autosampler Queue Buttons

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



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

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

The screenshot shows a spreadsheet titled 'Autosampler queue'. It has six columns: Num, Control file, Temperature file, Standard weight, Sample weight, and Recalib. le. The data is as follows:

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

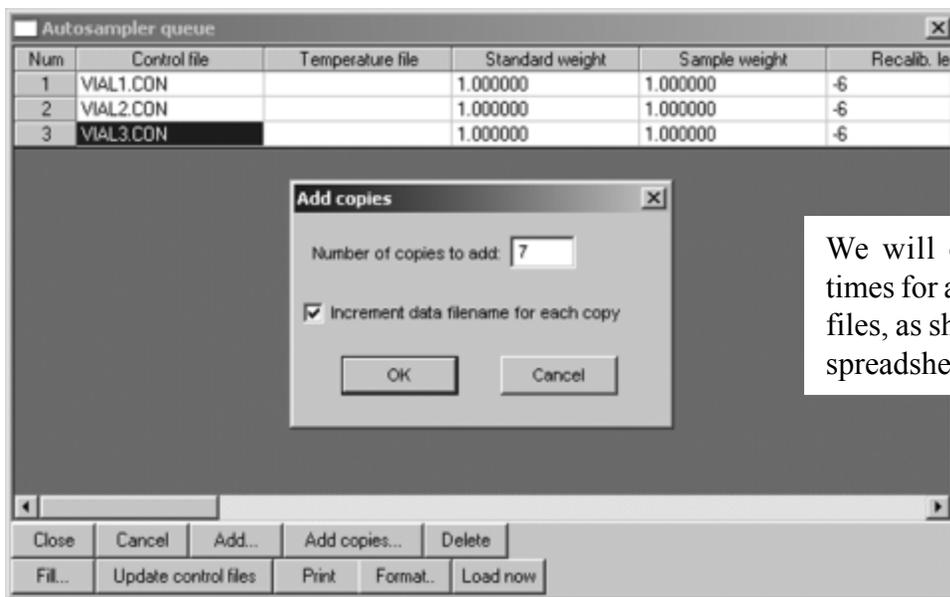
At the bottom of the window, there is a toolbar with buttons: Close, Cancel, Add..., Add copies..., Delete, Fill..., Update control files, Print, Format., and Load now.

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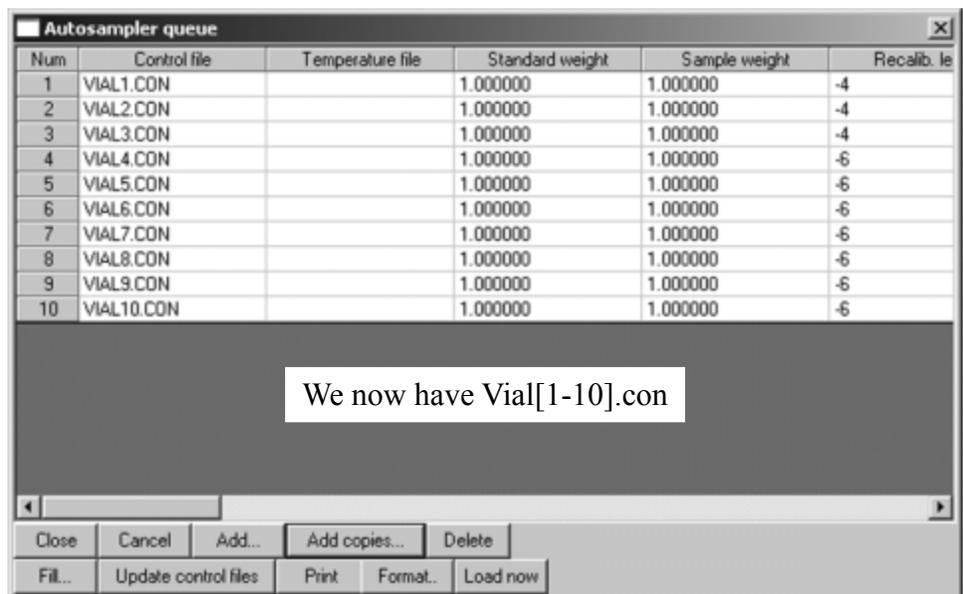
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Highlight the control file that is your master, or the one that is to be repeated, and click the “Add copies” button. In the window that pops up, enter the number of copies you wish to make, and check the “Increment data filename for each copy” box.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

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



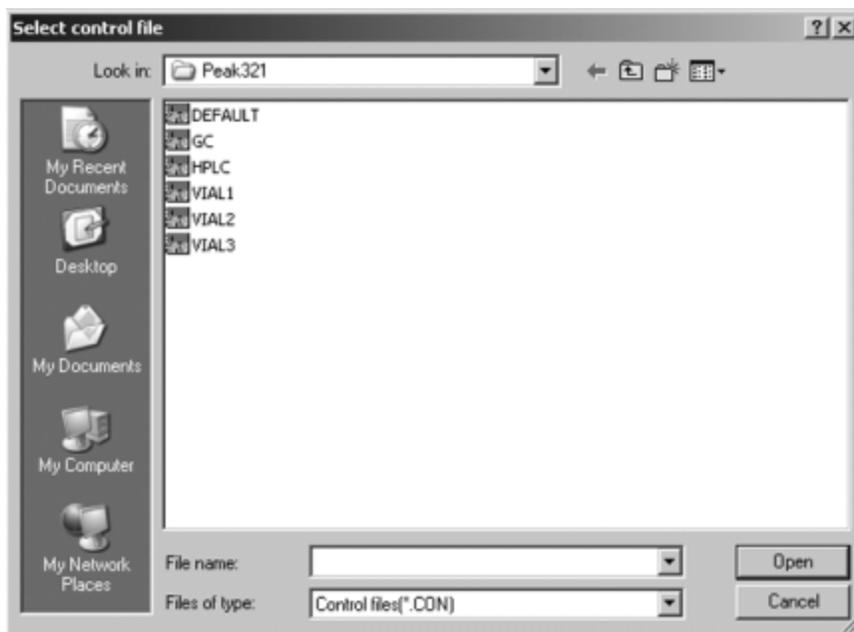
We will copy Vial3.con 7 times for a total of 10 control files, as shown in the Edit all spreadsheet below.



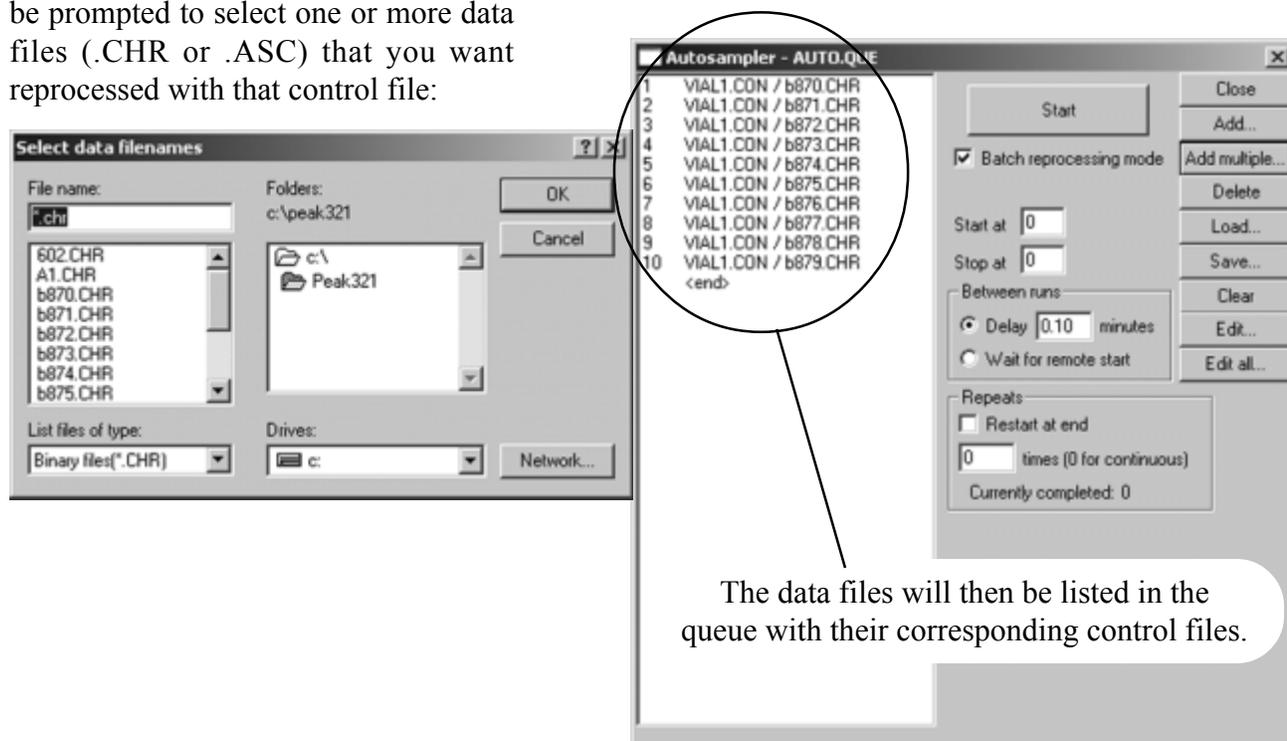
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The “Add multiple” button is for batch reprocessing. Batch reprocessing allows you to reprocess the raw data through a designated control file. This is useful in the event of a mistake or omission, or when header/comment info needs updating. The “Batch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

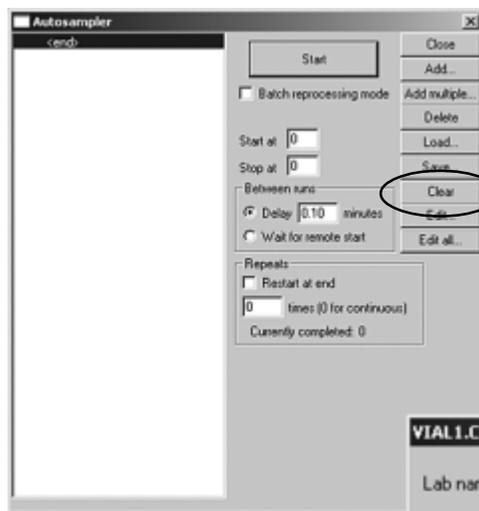
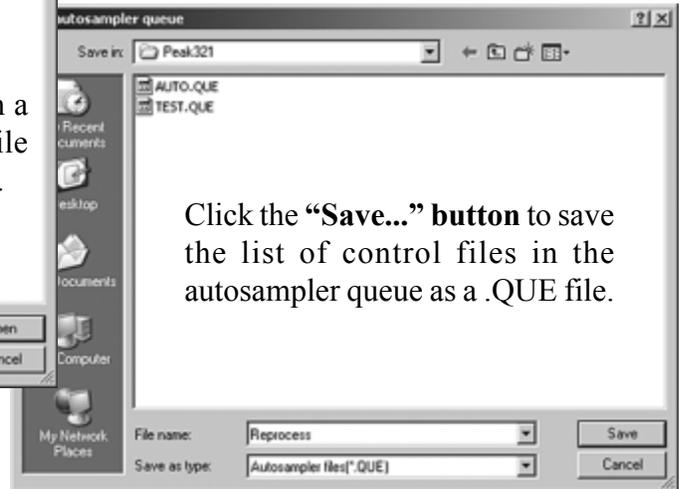
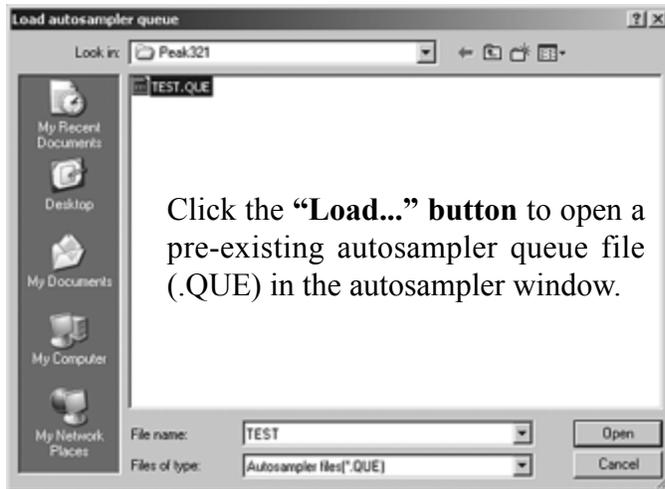


When you select a control file, you will be prompted to select one or more data files (.CHR or .ASC) that you want reprocessed with that control file:

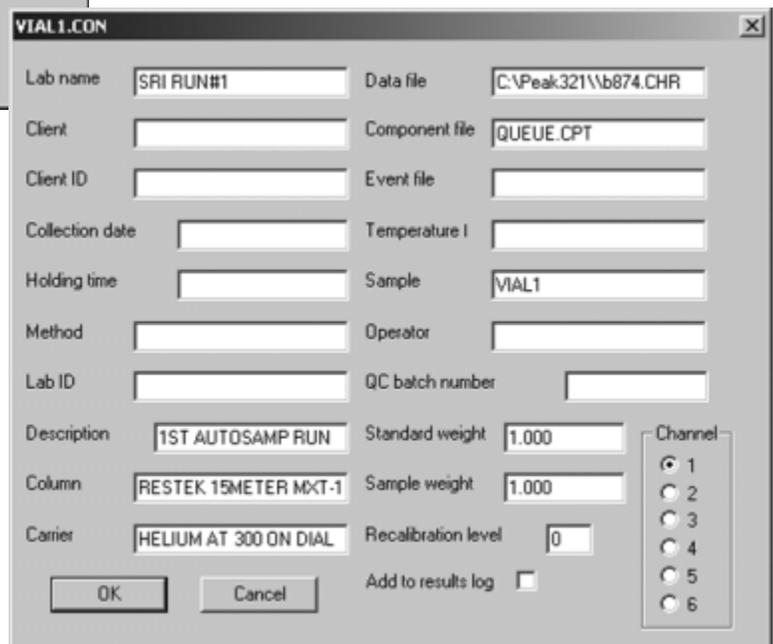


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To delete a control file from the autosampler queue, highlight it and click the **“Delete”** button. If no control file is highlighted, the last file in the list will be deleted when this button is clicked.



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

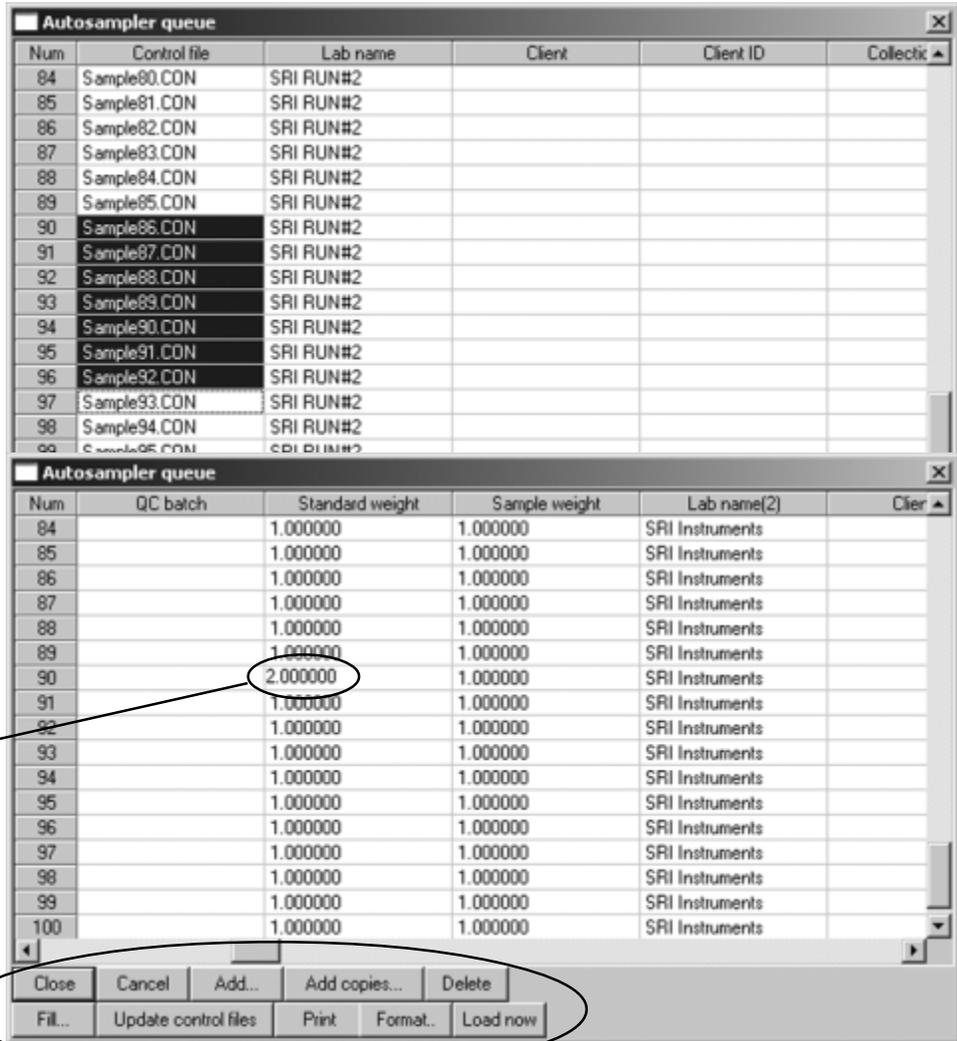


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Click on the “**Edit all...**” button to open the control file attributes spreadsheet. The Edit all spreadsheet is a powerful tool for managing your control files; it allows you to edit any or all of the control files in the autosampler queue.

You can highlight an entire column to change...



...Or make changes in individual cells.

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

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

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

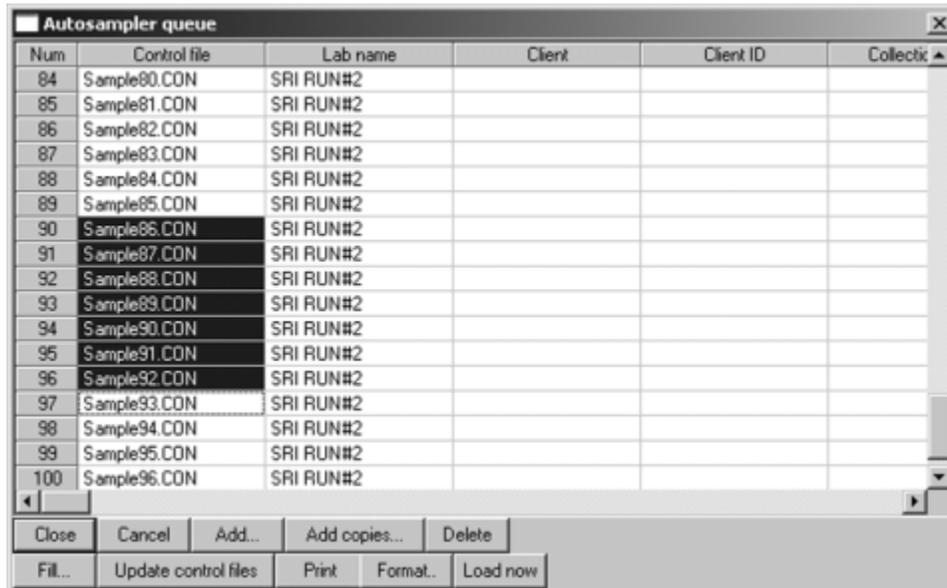
Click the “**Add...**” button to add a control file to the queue and spreadsheet.

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

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

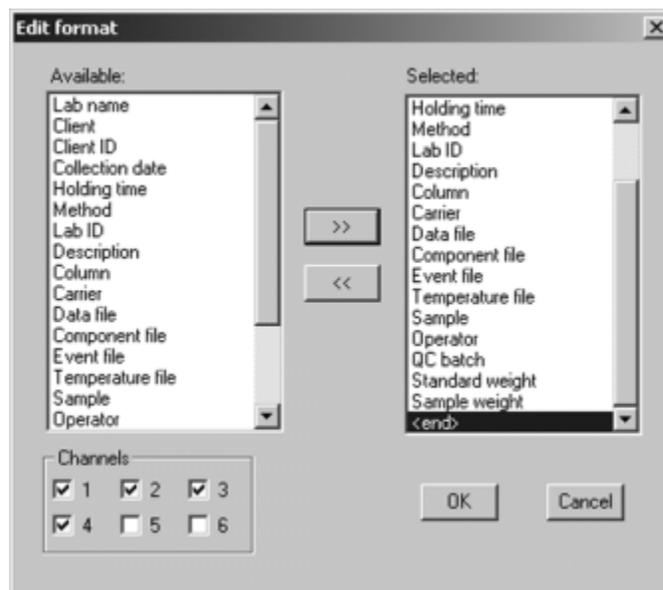
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Use the “**Fill...**” button after highlighting a vertical column in the spreadsheet to fill the cells with new text. To highlight a vertical column, click in the uppermost cell you want to include, then drag your cursor down to the last cell you want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



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

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



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

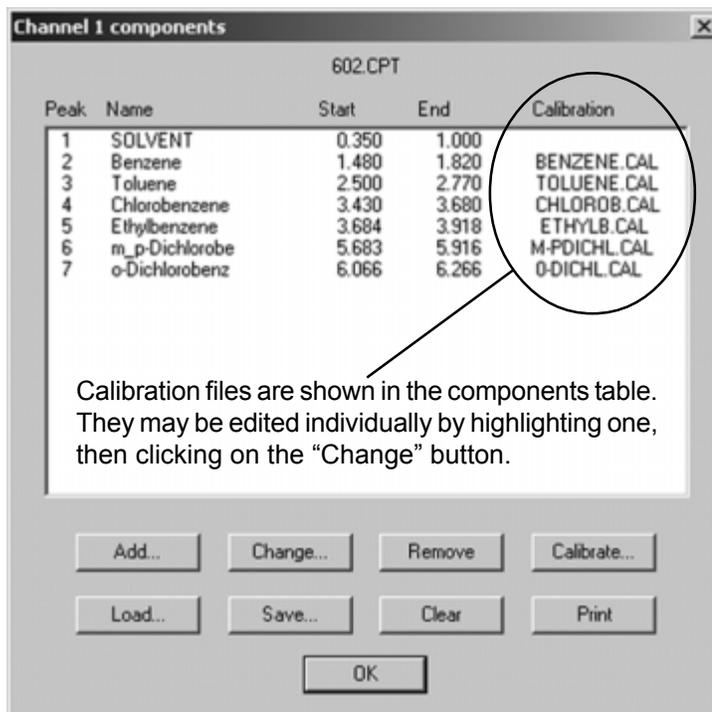
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Calibration

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

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



To make the first 3 vials calibration standards:

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

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

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

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

