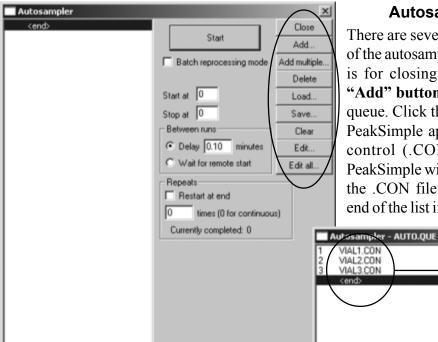
The Autosampler Queue is the most powerful and complex function of PeakSimple, and requires a throrough understanding of the software's features. If you are at the beginner level, you should not attempt to use this feature.

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.

🐺 PeakS	imple - COM1										_ 🗆 ×	
File Edit	View Acquisition	Help							Autosampler	_		×
	 Relay/pump wind 		1	2	3 4	5	6 速	2	<end></end>		Start	Close Add
1	3D display	N 3	/IAL2	2.CON								
1	30 display Channel 1 Channel 2 Channel 3 Channel 4 Channel 5 Channel 6 Unzoom Refresh	F9 F10 F11 F12 F6 Enter	/AL2	2.CON							Batch reprocessing mode Start at 0 Stop at 0 Between runs © Delay 0.10 minutes © Wait for remote start Repeats Restart at end 0 times (0 for continuou Currently completed: 0	Add multiple Delete Load Save Clear Edit Edit all
	10.000											
	4 4 4 0.000							_			1.000	

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



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

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

Autosampler queue X Num Control file Temperature file Standard weight Sample weight Recalib. le VIAL1.CON 1 1.000000 1.000000 -2 VIAL2.CON 1.000000 1.000000 -2 2 1.000000 VIAL3.CON 1.000000 .2 3 4 F Cancel Add. Delete Close Add copies.. Fill. Update control files Print Format. Load now

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).

Start

Batch reprocessing mode

Delay 0.10 minutes

times (0 for continuous)

C Wait for remote start

Currently completed: 0

Start at 0

Stop at 0

Repeats Restart at end

0

Between runs

×

Add

Delete

Load.

Save.

Clear

Edit

Edit all.

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.

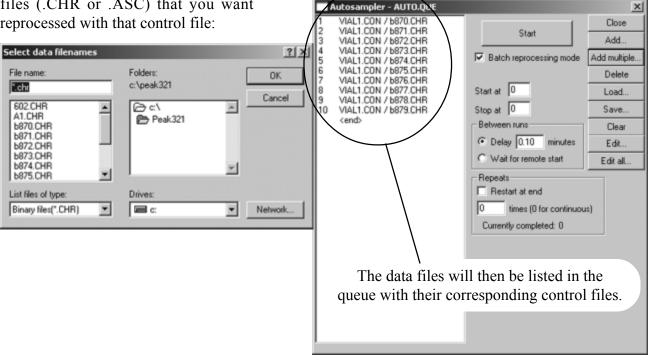
Aut	osampler queue				×	
Num	Control file	Temperature file	Standard weight	Sample weight	Recalib. le	
1	VIAL1.CON		1.000000	1.000000	-6	
2	VIAL2.CON		1.000000	1.000000	-6	
3	VIAL3.CON		1.000000	1.000000	-6	
		Add copies Number of copies I Increment data OK	to add: 7 filename for each copy Cancel	×	times for a	copy Vial3.con 7 total of 10 control own in the Edit all et below.
•					<u>)</u>	
Close	Cancel Add	Add copies	Delete			
Fil	Update control files	Print Format.	Load now			

Aut	osampler queue				X
Num	Control file	Temperature file	Standard weight	Sample weight	Recalib. le
1	VIAL1.CON		1.000000	1.000000	-4
2	VIAL2.CON		1.000000	1.000000	-4
3	VIAL3.CON		1.000000	1.000000	-4
4	VIAL4.CON		1.000000	1.000000	-6
5	VIAL5.CON		1.000000	1.000000	-6
6	VIAL6.CON		1.000000	1.000000	-6
7	VIAL7.CON		1.000000	1.000000	-6
8	VIAL8.CON		1.000000	1.000000	-6
9	VIAL9.CON		1.000000	1.000000	-6
10	VIAL10.CON		1.000000	1.000000	-6
		We now ha	ve Vial[1-10].	con	
•					•
Close	Cancel Add	Add copies	Delete		
Fil	Update control files	Print Format.	Load now		

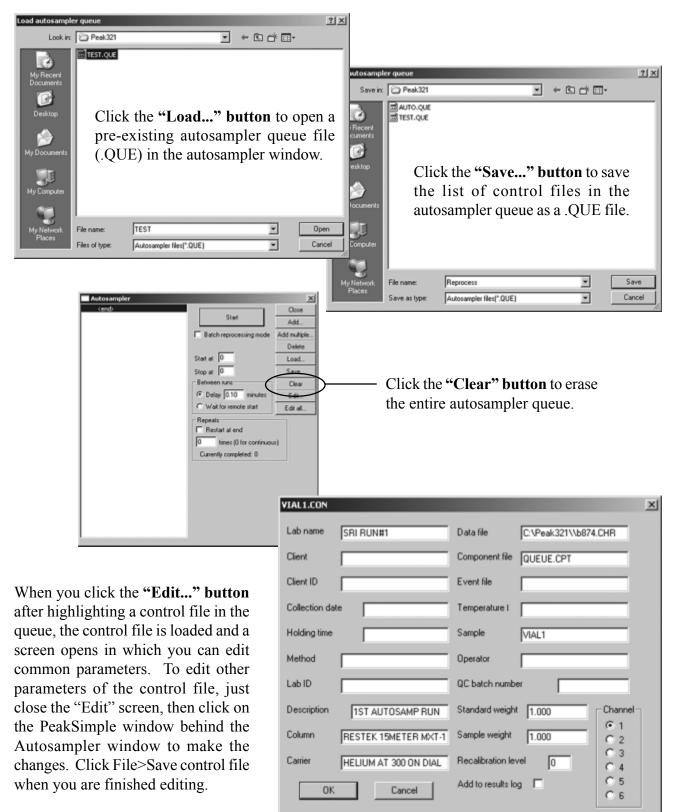
The "Add multiple" button is for batch reprocessing. Batch reprocessing allows you to reprocess the raw data through a designated control file. This is useful in the event of a mistake or omission, or when header/comment info needs updating. The "Batch reprocessing mode" checkbox to the left of the "Add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

Select control fil	e				<u>? ×</u>
Look in:	Peak321		•	← 🗈 💣 💷•	
My Recent Documents Desktop My Documents My Computer	33 DEFAULT 35 GC 35 HPLC 35 VIAL1 35 VIAL2 35 VIAL3				
My Network Places	File name:			*	Open
	Files of type:	Control files(".CDN)		-	Cancel

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:



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.



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

he autosampler queue.	Aut	osampler queue				1
	Num	Control file	Lab name	Client	Client ID	Collectic
	84	Sample80.CON	SRI RUN#2			
	85	Sample81.CON	SRI RUN#2			
	86	Sample82.CON	SRI RUN#2			
	87	Sample83.CON	SRI RUN#2			
	88	Sample84.CON	SRI RUN#2			
	89	Sample85.CON	SRI RUN#2			
		Sample86.CON	SRI RUN#2			
You can highlight an	91	Sample87.CON	SRI RUN#2			
	92	Sample88.CON	SRI RUN#2			
entire column to		Sample89.CON	SRI RUN#2			
change	94	Sample90.CON	SRI RUN#2			
	95	Sample91.CON	SRI RUN#2			
		Sample92.CON	SRI RUN#2			
	97	Sample93.CON	SRI RUN#2			
	98	Sample94.CON	SRI RUN#2			
	00	Campion 30alanas 2	CDI DI IN#2			
		osampler queue				
	Num 84	QC batch	Standard weight	Sample weight	Lab name(2)	Clier
	84		1.000000 1.000000	1.000000	SRI Instruments SRI Instruments	
	85		1.000000	1.000000		
	87		1.000000	1.000000	SRI Instruments	
	88		1.000000	1.000000	SRI Instruments SRI Instruments	
	89		1.000000	1.000000	SRI Instruments	
	90		(2.000000)	1.000000	SRI Instruments	
	91		1.000000	1.000000	SRI Instruments	
.Or make changes in	- 92		1.000000	1.000000	SRI Instruments	
	93		1.000000	1.000000	SRI Instruments	
ndividual cells.	94		1.000000	1.000000	SRI Instruments	
	- 34		1.000000	1.000000		
	95		1.000000	1 000000	CDI Instrumente	
	95		1.000000	1.000000	SRI Instruments	
	96		1.000000	1.000000	SRI Instruments	
	96 97		1.000000 1.000000	1.000000 1.000000	SRI Instruments SRI Instruments	
	96 97 98		1.000000 1.000000 1.000000	1.000000 1.000000 1.000000	SRI Instruments SRI Instruments SRI Instruments	
	96 97 98 99		1.000000 1.000000 1.000000 1.000000	1.000000 1.000000 1.000000 1.000000	SRI Instruments SRI Instruments SRI Instruments SRI Instruments	
	96 97 98		1.000000 1.000000 1.000000	1.000000 1.000000 1.000000	SRI Instruments SRI Instruments SRI Instruments	
	96 97 98 99 100 ▼	Cancel Add	1.000000 1.000000 1.000000 1.000000 1.000000	1.000000 1.000000 1.000000 1.000000 1.000000	SRI Instruments SRI Instruments SRI Instruments SRI Instruments	1
	96 97 98 99	Cancel Add	1.000000 1.000000 1.000000 1.000000 1.000000 Add copies	1.000000 1.000000 1.000000 1.000000	SRI Instruments SRI Instruments SRI Instruments SRI Instruments	Ľ

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.

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

Num	Control file	Lab name	Client	Client ID	Collectic A
84	Sample80.CON	SRI RUN#2			
85	Sample81.CON	SRI RUN#2			
86	Sample82.CON	SRI RUN#2			
87	Sample83.CON	SRI RUN#2			
88	Sample84.CON	SRI RUN#2			
89	Sample85.CON	SRI RUN#2			
90	Sample86.CON	SRI RUN#2			
91	Sample87.CON	SRI RUN#2			
92	Sample88.CON	SRI RUN#2			
93	Sample89.CON	SRI RUN#2			
94	Sample90.CON	SRI RUN#2			
95	Sample91.CON	SRI RUN#2			
96	Sample92.CON	SRI RUN#2			
97	Sample93.CON	SRI RUN#2			
98	Sample94.CON	SRI RUN#2			
99	Sample95.CON	SRI RUN#2			
100	Sample96.CON	SRI RUN#2			
					•
Close	Cancel Add	d Add copies	Delete		
Fil	Update control file	es Print Format.	Load now		

Click the "Update control files" button to save all the changes made to the control files in the spreadsheet.

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

Edit format	×
Available:	Selected: Holding time Method Lab ID Description Column Carrier Data file Component file E vent file E vent file Sample Operator QC batch Standard weight Sample weight Sample weight Vendo
Channels ↓ 1 ↓ 2 ↓ 3 ↓ 4 ↓ 5 ↓ 6	OK Cancel

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.

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 calibrations 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

hannel	1 components			×
		602.CPT		\frown
Peak	Name	Start	End	Calibration
Т	SOLVENT Benzene Toluene Chlorobenzene Ethylbenzene m_p-Dichlorobe o-Dichlorobenz calibration files are hey may be edited nen clicking on th	d individua	ally by high	nlighting one,
Ľ	Add Char	nge	Remove	Calibrate
Γ	Load Sav	/e	Clear	Print
		ОК		

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.

Channel 1 post-run actions
Save file as: A1.CHR
Save results Add to results log: CH1.LOG
Print results Update DDE link
Execute:
Restart run after: 10.00 minutes 0 times total (0 remaining)
Recalibrate at level 1 Save results file to FTP site
Smooth first Save data file to FTP site
Copy data to channet
Add to 3D display
OK Cancel