MassLynx NT Guide to Inlet Control

Version 3.5

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MassLynx NT Guide to Inlet Control

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Controlling Inlet Systems and Autosamplers

Chapter 1

Introduction

Mass spectrometers are usually used in conjunction with an inlet system such as a liquid chromatograph (LC) or a gas chromatograph (GC). MassLynx can control this equipment during data acquisition to provide complete control of an experiment. Autosamplers will often be used to automate the running of samples.

Inlets

Acquisitions that use an inlet system can only be started from the Instrument Control Panel and cannot be started from the tune page. Before you try to use an inlet system for the first time you must configure MassLynx to use that inlet. To select a new inlet system, choose **Select Interface** from the Acquisition Control Panel **Configure** menu.

The list of inlet options that appears in the Select Interface dialog reflects the inlet systems, which were selected when MassLynx was installed. For some Inlet systems (HP1090, HP1050, HP1100, HP6890, Jasco, Waters, MicroTech and Gilson) selecting the **GC or LC system (ACE)** (Analytical Component Engine) option allows the user to change the Inlet, Autosampler and Detector without having to re-install MassLynx. For other non ACE systems if, at a later date you add a new inlet system or change one of your existing inlets you may need to re-install MassLynx to gain access to the control software for the new inlet system.

The method used to control the inlet system is set up before you start to acquire any data and is saved on disk for use by the acquisition system. Different methods can be saved, accessible by name in the usual manner. You must supply the name of the inlet method that you wish to use when you start an acquisition by entering it into the 'Inlet' field in either the Single or Multiple sample start editors (these are covered in the next section).

N.B. Make sure that any changes that you make to an inlet program are saved to disk before you start an acquisition. This is done by selecting the Save option on the File menu of the inlet editor or by pressing the  toolbar button. If you do not save the parameters then the previous ones will be used as MassLynx reads the parameters from disk, not from the editor, when it starts to acquire. Iconising the display does **not** save the parameters but you will be given the option to save any changes that you have made if you actually close the editor.

Autosamplers

An autosampler can only be used with the multiple sample acquisition editor on the MassLynx top level screen.

The rules regarding the saving of parameters for inlet editors apply to autosampler editors as well.

The Inlet Editor

The Inlet Editor is used to

- View the status of the current system.
- Define the GC or LC, autosampler and detector methods.
- Change instrument configuration
- Control pumps and lamps and run methods.

To access the Inlet Editor press the  toolbar button on the LC panel of the MassLynx top level screen, or select **Inlet** from the **Methods** menu on the Acquisition Control Panel.

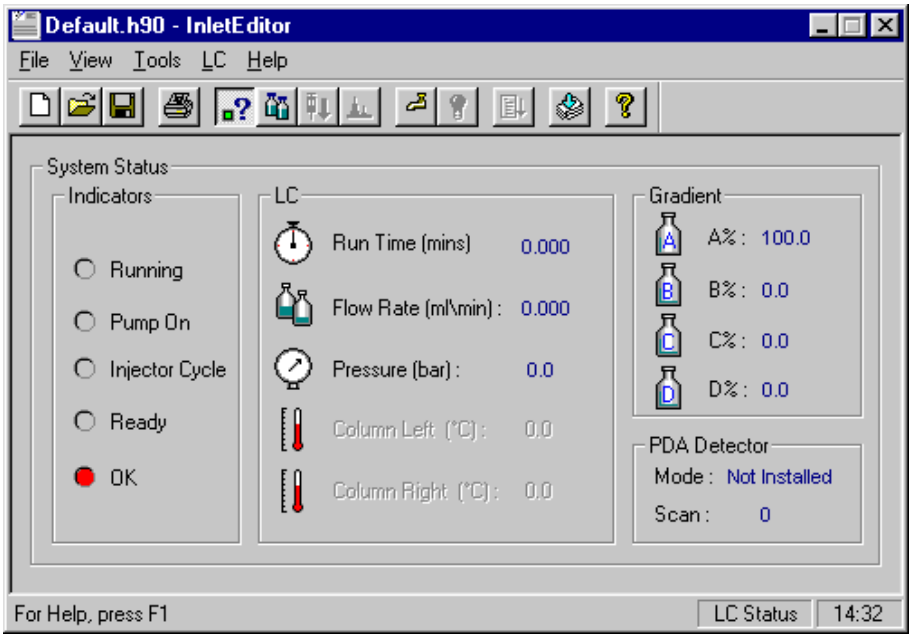


Figure 1.1 *Inlet Editor dialog – System Status page*

The Inlet Editor Toolbar

The toolbar is displayed across the top of the application window, below the menu bar. The toolbar provides quick mouse access to many tools used in the control software.

Click	To
	Create a New method.
	Open an existing method.
	Save the method with its current name.
	Print the current method.
	Display the System Status dialog.
	Edit Inlet system parameters.
	Edit AutoSampler parameters.
	Edit Detector parameters.
	Start or stop the pump.
	Turn Lamp on and off.
	Run the currently saved method
	Load the currently saved method.
	Display the Help Contents.

The System Status Page

The System Status page displays information about the state of the machine being controlled. This page can be accessed within the Inlet Editor by selecting **Status** from the **View** menu or by pressing the  toolbar button. **Note**: This changes for a GC, see HP6890 later in the manual. The Waters Cap LC also has a different System Status page see the Waters Cap LC System Status Page later in this chapter.

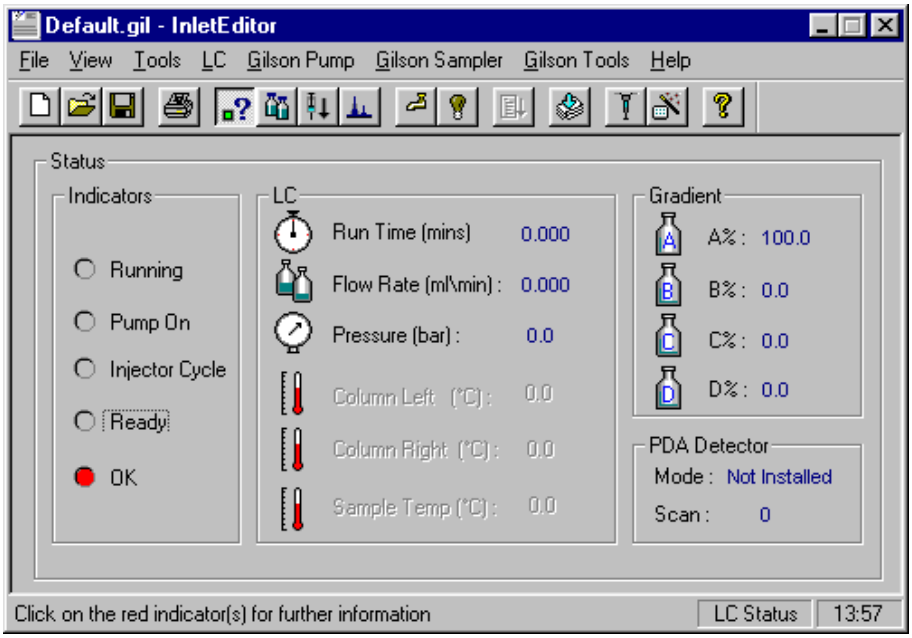


Figure 1.2 *System Status page*

Indicators The Running, Pump On and Injector Cycle indicators at the left-hand side of the screen give you information on the current status of the LC system. The OK and Ready Indicators become illuminated in red if the LC System has an error. You can then click on the red indicators to give you more information on the cause of the malfunction.

Run Time Displays how long the method has been running.

Flow Rate This is the current flow rate as returned by the instrument.

Pressure Displays the current pressure in the instrument.

Column Left and **Column Right** Displays the current temperature of the left and right columns. These will be grayed out if column heaters are not installed.

Sample Temp Displays the current temperature of the sample. This will be grayed out if a sample heater is not installed.

Gradient Displays the solvent percentages at which the LC System is currently operating.

PDA Detector When acquiring diode array data the Diode Array Status displays the number of scans currently acquired.

- **Saving and loading LC parameter files**

  The Current LC parameters can be saved to disk by choosing **Save** or **Save As** from the Inlet Editor **File** menu.

  A set of previously saved LC parameters can be recalled from disk by choosing **Open** from the Inlet Editor **File** menu.

- **To print an LC Method Report**

  Choose **Print** from the Inlet Editor **File** menu or press the  toolbar button. Press **OK** to print a report detailing the parameters used in the current LC Method.

- **To Download parameters to the LC system**

  To download the parameters to the LC system, press the  button or choose **Load Method** from the **LC** menu.

  The status bar will indicate the progress of downloading the parameters. Once values have been downloaded you can start the pump running with the initial conditions.

- **To Run the Pump with initial conditions**

  Select **Pump On** from the **LC** menu or click on the  button. The pump will begin running with its initial conditions.

- **To turn on the Lamp**

  Select **Lamp On** from the **LC** menu or click on the  button.

- **To begin a Gradient Method or start an injection**

  You can run a single injection with the Autosampler by selecting **Run Method** from the **LC** menu as soon as the menu item is enabled (it is disabled when the system is running a method). If a method is already running in the LC System it will not be possible to start a new method (either inject or run gradient only) until the previous method has stopped.

  Selecting **Run Method (No Injection)** from the **LC** menu starts the gradient (if entered) to allow manual injections.

Inlet Configuration

As mentioned earlier selecting the **GC or LC system (ACE)** option, from the Select Interface dialog, allows the user to change the Inlet, Autosampler and Detector without having to re-install MassLynx. The Inlet Configuration dialog gives a list of the Inlet systems, Autosamplers and detectors supported by MassLynx. To access the dialog select **Instrument Configuration** from the **Tools** menu on the Inlet Editor.

Instruments

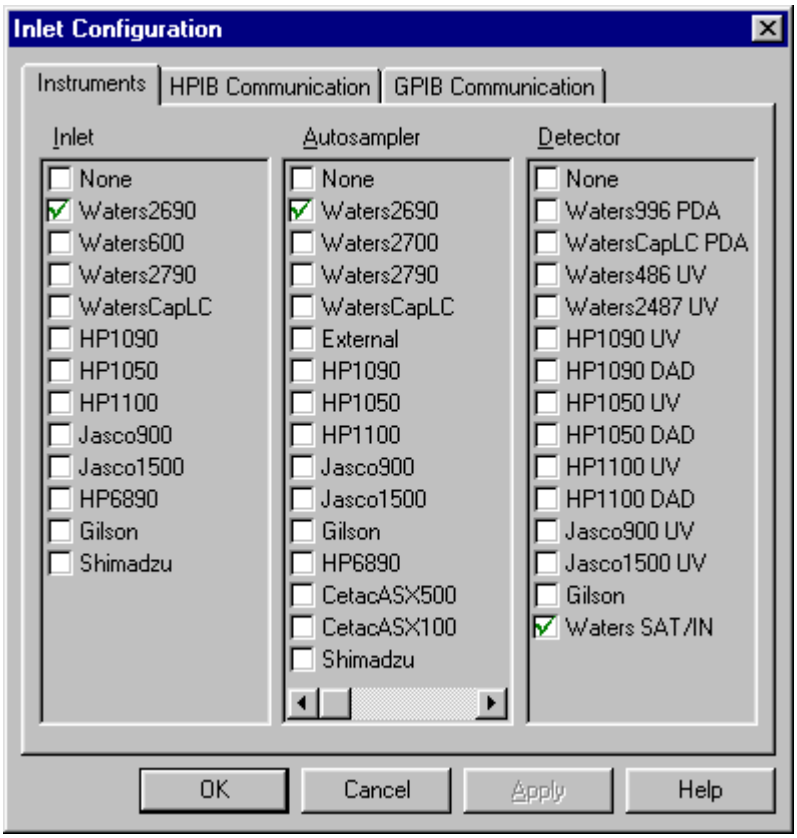


Figure 1.3 *Instrument Configuration dialog*

Check the boxes for the required configuration and press OK. MassLynx will inform the user if the configuration is not supported.

HPIB Communication

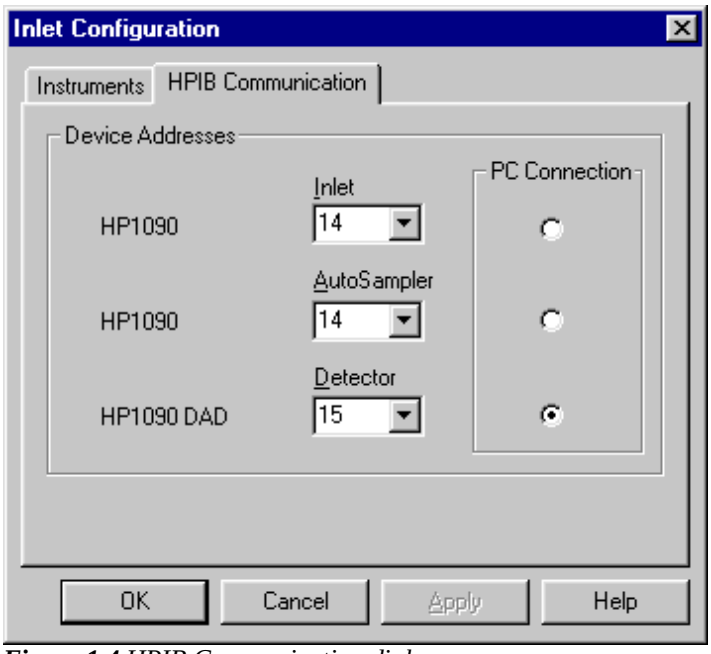


Figure 1.4 *HPIB Communication dialog*

When an Instrument configuration has been selected on the Instrument tab default device addresses are written to this dialog. Values can be changed if required. For the HP1100 DAD detector the PC Connection should be set to HP100 DAD.

GPIB Communication

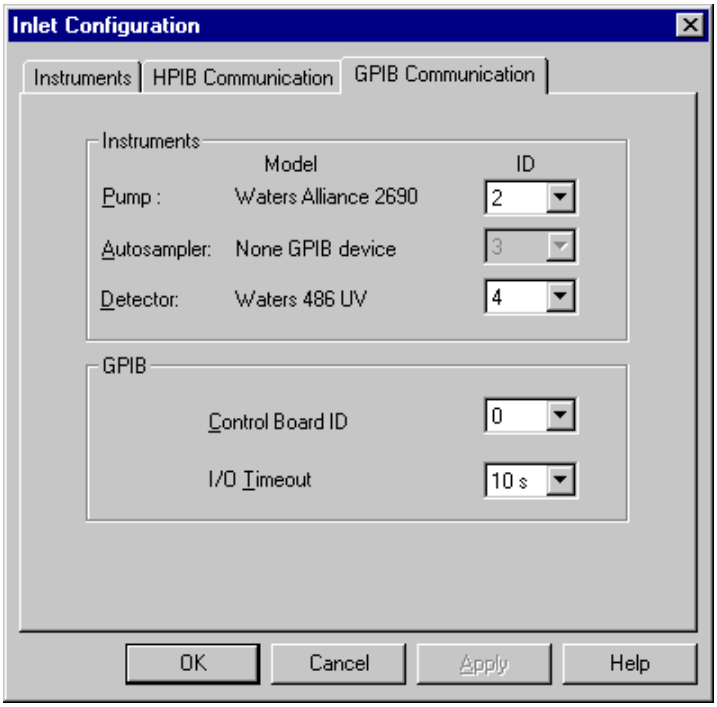


Figure 1.5 *GPIB Communication dialog*

When an Instrument configuration has been selected on the Instrument tab default IDs are written to this dialog. These may need changing and will be defined on setup by a Micromass engineer. For more information consult the relevant instrument instruction manual.

Notes

Notes

Waters Systems

Chapter 2

Waters 600 Pump

The Waters 600 Pump pages can be accessed by selecting **Waters600 Pump** from the **View** menu on the Inlet Editor or by pressing the  toolbar button.

- **Waters 600 Initial Conditions**

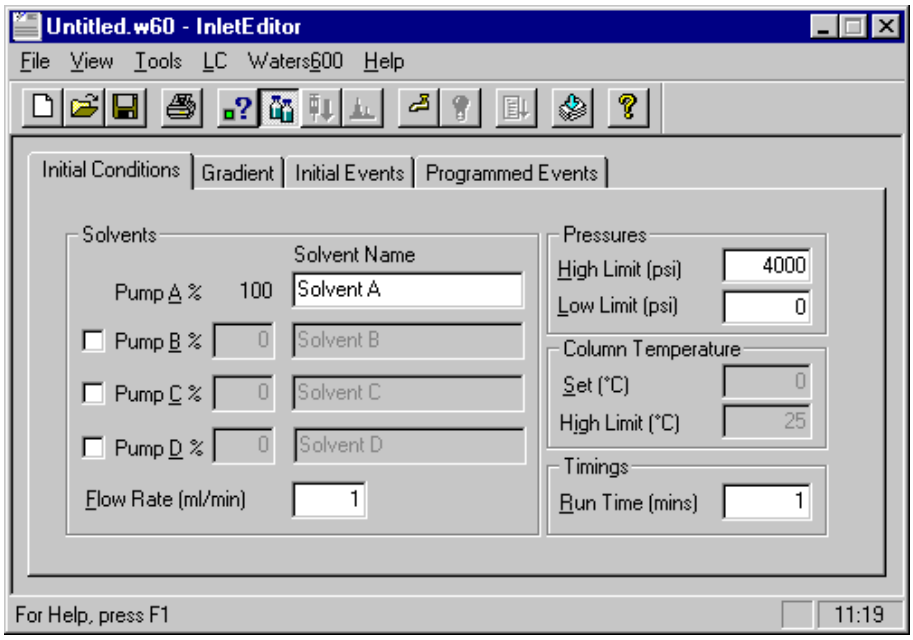


Figure 2.1 *Initial Conditions page*

Solvents Up to four solvents will be displayed depending upon the system configuration. The total value of all the solvent percentages added together must not exceed 100%.

Pump A This is the remainder percentage after the solvent percentages have been set for the other pumps.

Pump B, C and **D** These can either be enabled or disabled by checking the box next to the individual pumps. The values can be set to the required percentage of flow delivery.

Solvent Name Enter the name of the solvent that will be delivered through the corresponding Pump.

Flow Rate This is the total flow rate of the solvent channels according to how you have configured the instrument.

Pressures Enter the upper and lower limits of the pressure within the solvent delivery system (SDS) if the pressure falls outside of this range the SDS switches off.

Column Heater If the instrument has an oven present then the column temperature can be set to a specified temperature in degrees centigrade. Enter the temperature to heat the column to in the **Set** box and a **High Limit**. If the temperature exceeds the High Limit then the system will shut down. If the software has been configured to operate without a column oven then these boxes will be greyed out.

Run Time Enter the time in minutes that the method will run from the point of injection.

- **Waters 600 Gradient Page**

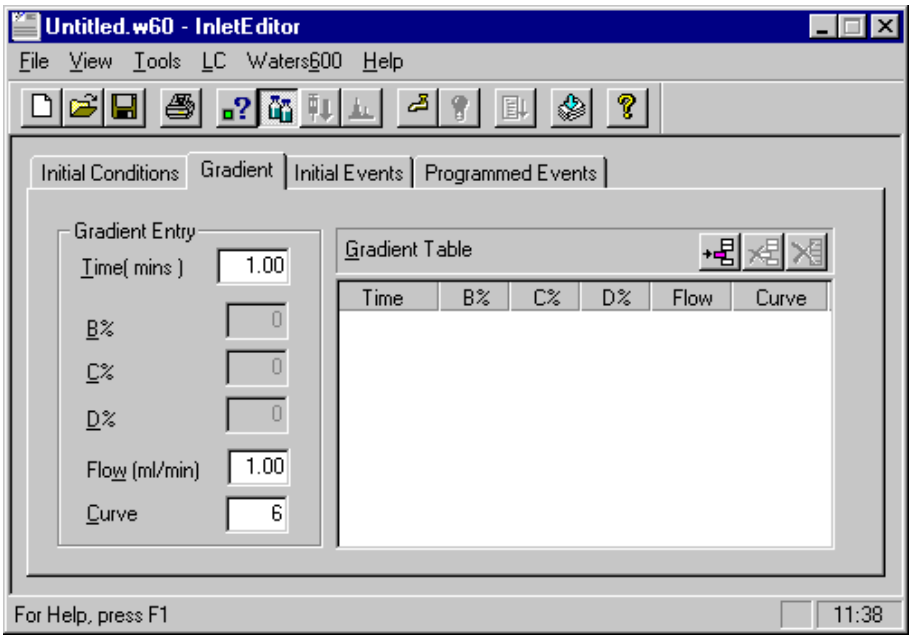


Figure 2.2 *Gradient page*

This page allows a gradient to be entered and edited. To operate in isocratic mode ensure that the timetable is empty.

To enable the **B%**, **C%** and/or **D%** boxes check the relevant boxes on the **Initial Conditions** page.

To add a gradient, enter a time and percentage in the relevant boxes and press the  toolbar button. **Note:** The first entry must have a time of 0.

To delete a single gradient, click with left mouse button on a time in the list and press the  toolbar button.

To delete all entries press the  toolbar button. This button is only available when there are entries in the timetable.

To modify a gradient, select the required entry in the timetable. The values will then be displayed in the edit boxes to the left of the timetable, and can be altered as appropriate. Once changed press  to re-enter the values into the timetable. If, however, you modify the time value such that it does not correspond to any existing entry in the timetable pressing  will result in a new entry being created in the timetable.

Flow Enter the flow rate for the solvent delivery system.

Curve This sets the rate at which the solvent is to change to the new proportions and/or flow rates. See the Waters 600 Operator's Guide for a list of values.

Waters 600 Initial Events Page

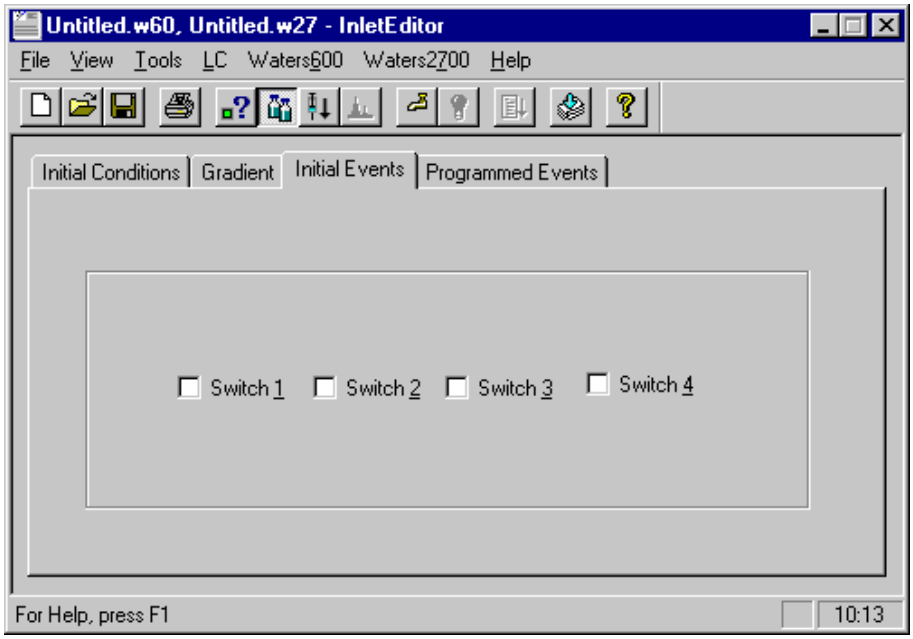


Figure 2.3 *Initial Events page*

This page allows the initial state of switches 1 to 4 to be defined. Check the box(es) for the switches that should have an initial state of off.

Waters 600 Programmed Events Page

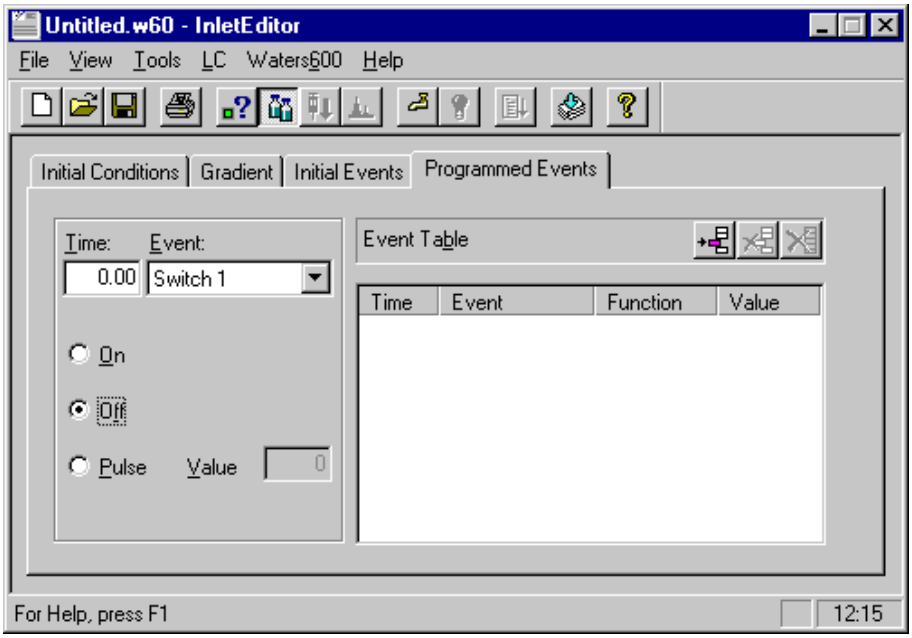


Figure 2.4 *Programmed Events page*

This page allows pump events to be entered and edited.

To add an event, type in a time, select an event from the drop down list box, select an action or enter a value and press the  toolbar button.

To delete a single event, click with left mouse button on a time in the list and press the  toolbar button.

To delete all entries press the  toolbar button. This button is only available when there are entries in the timetable.

To modify an event, select the required entry in the timetable. The values will then be displayed in the edit boxes above the timetable, and can be altered as appropriate. Once changed press  to re-enter the values into the timetable. If, however, you modify the time value such that it does not correspond to any existing entry in the timetable pressing  will result in a new entry being created in the timetable.

Waters 2690 Autosampler

Note: To control the Waters 2690 autosampler and pump from the keypad rather than the MassLynx software the **Inlet** must be configured as **None**. See Configuring the Inlet System in the Acquisition Control Panel chapter.

Waters 2690 Autosampler Initial Conditions Page

This page is used to set parameters specific to the Sampler, to access it select **Waters2690 AutoSampler** from the **View** menu or press the  toolbar button.

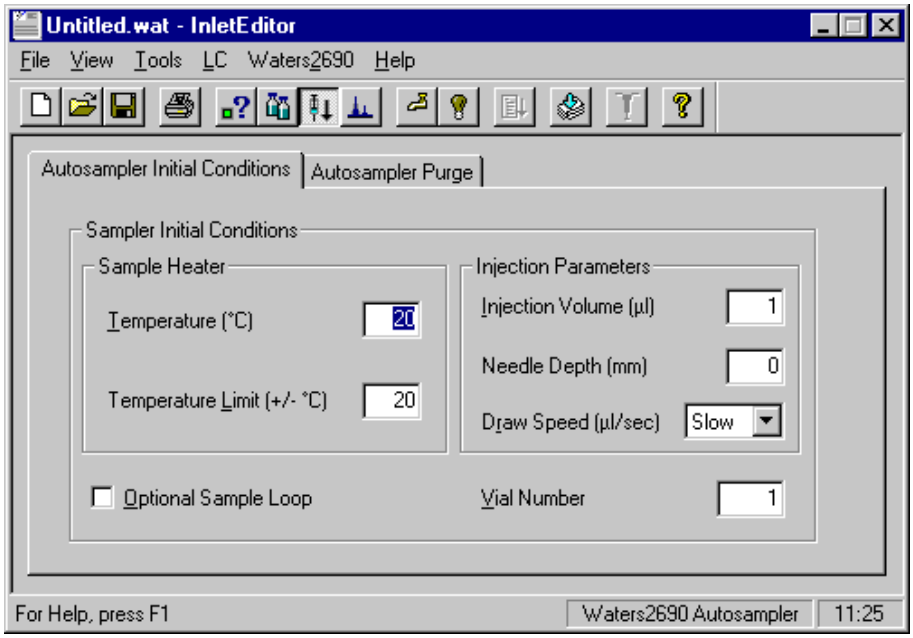


Figure 2.5 *Autosampler Initial Conditions page*

Sample Heater Temperature If the sample heater is installed, enter the temperature that the sample should be to be heated or cooled to.
Range: 4.0 to 40.0 °C.

Sample Heater Temperature Limit Enter the maximum deviation in sample temperature allowed. If this is exceeded the current acquisition will stop and the LC Status error light, on the MassLynx screen, will turn red. Range: ±1.0 to ±20.0 °C.

Injection Volume Enter the volume of sample to be injected, in microlitres. Range: 0 to 2000 µl. **Note:** If you are running from the Sample List, the injection volume in the sample list entry overrides the value entered here.

Needle Depth This adjusts the depth of the needle tip to accommodate for sedimented samples or non-standard vials. A value of 0 corresponds to the bottom of the vial. Range: 0.0 to 20.0 mm in 0.1mm increments.

Draw Speed This determines the rate in microlitres per second at which sample is extracted into the autosampler needle. It should be set according to the viscosity of the sample. Select one of **Fast**, **Normal** or **Slow** from the dropdown list box. The table below shows the draw rate for each selection using a 250 µl syringe.

Selection	Draw Rate for a 250 µl Syringe
Fast	5.0 µl/sec
Normal	2.5 µl/sec
Slow	1.0 µl/sec

Optional Sample Loop To inject sample volumes greater than 100 microlitres an additional sample loop can be installed (in series with the existing sample loop), check this box if an additional sample loop is used.

Vial number The vial to inject from. **Note:** If a multisample acquisition is being run from the MassLynx Sample List, the Bottle # entry in the sample list overrides the value entered here.

Waters 2690 Autosampler Purge Page

This page is used to set the Autosampler purge volume, to access it click on the Autosampler Purge tab.

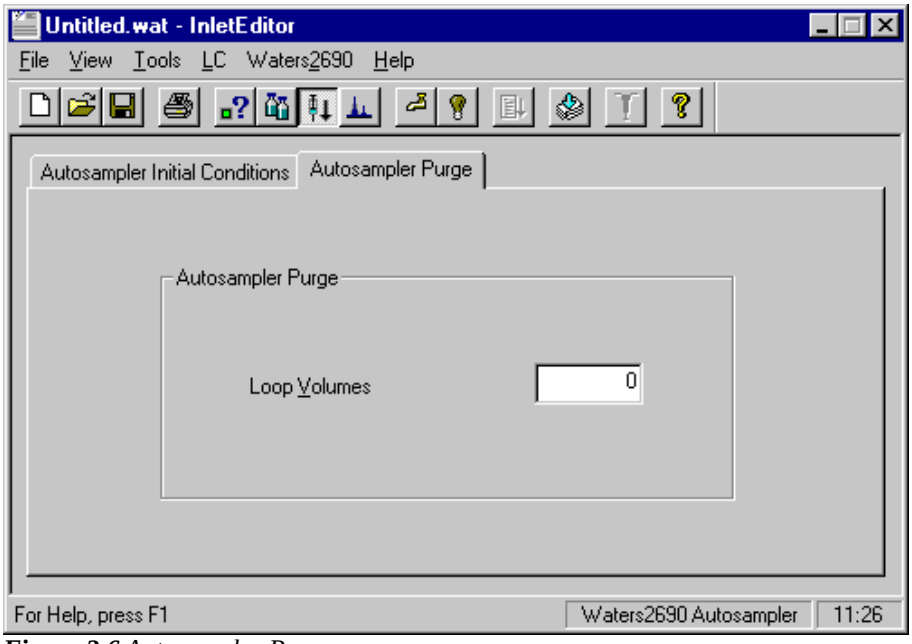


Figure 2.6 *Autosampler Purge page*

Loop Volumes Enter the number of times the loop should be filled to purge the sample loop and syringe of traces of the previous sample. When set to a value greater than zero, this action is performed after every injection.

Waters 2690 Pump

Note: To control the Waters 2690 autosampler and pump from the keypad rather than the MassLynx software the **Inlet** must be configured as **None**. See Configuring the Inlet System in the Acquisition Control Panel chapter.

The Waters Pump pages can be accessed by selecting **Waters2690 Pump** from the **View** menu on the Inlet Editor or by pressing the  toolbar button.

Waters 2690 Solvents and Flows Page

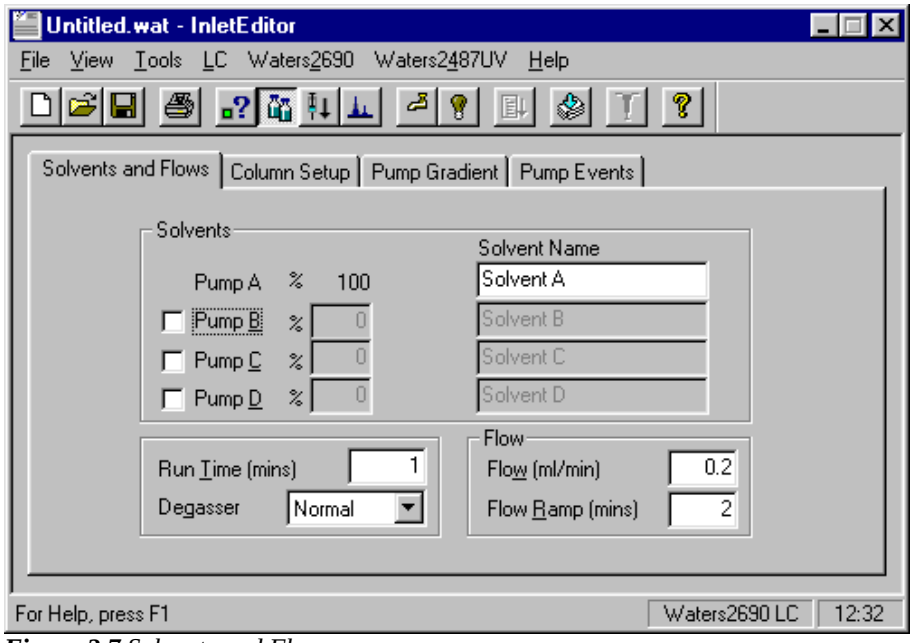


Figure 2.7 *Solvents and Flows page*

Solvents Up to four solvents will be displayed depending upon the system configuration. The total value of all the solvent percentages added together must equal 100%. Solvent Names entered here will be displayed on the Pump Gradient page.

Pump A This displays the remainder percentage after the solvent percentages have been set for the other enabled pumps.

Pump B, C and **D** These can either be enabled or disabled by checking the box next to the individual pumps. The values can be set to the required percentage of flow delivery.

Run Time This value is set to the time in minutes that the method will run from the point of injection.

Degasser This value is set to the time in minutes that the method will run from the point of injection.

Flow This is the total flow rate for the system.

Flow Ramp Enter the time (in minutes) for the solvent delivery system to reach the maximum system flow rate (10 ml/min). Recommended minimum setting: 0.5 min.

- **Waters 2690 Column Setup Page**

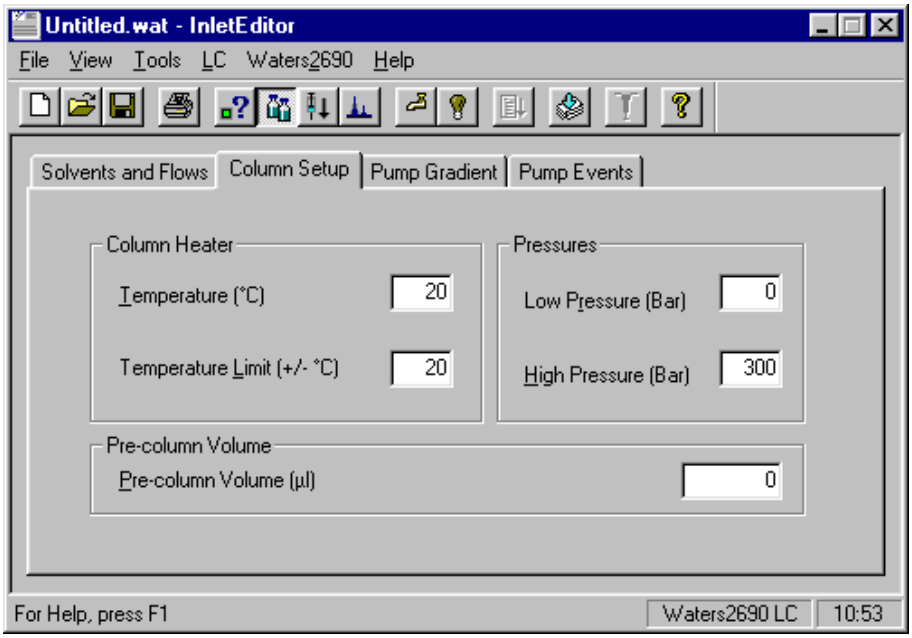


Figure 2.8 *Column Setup page*

Column Heater Temperature Enter the target operating temperature for the optional column heater. This value must be at least 5 °C above ambient. Range: 20 to 60 °C.

Column Heater Temperature Limit This is the maximum deviation in column temperature allowed. If this is exceeded the current acquisition will stop and the LC Status error light, on the MassLynx screen, will turn red. Range: ±1 to ±20 °C.

Enter **Low Pressure** and **High Pressure** values as required. If the pressure falls outside these limits the current acquisition will stop and the LC Status error light, on the MassLynx screen, will turn red. Low Pressure Range: 0 to 310 bar. Low Pressure Range: 0 to 345 bar.

Pre-column Volume Enter the volume of solvent to pump through the column before an injection. Range: 1 to 10000 µl.

Waters 2690 Pump Gradient Page

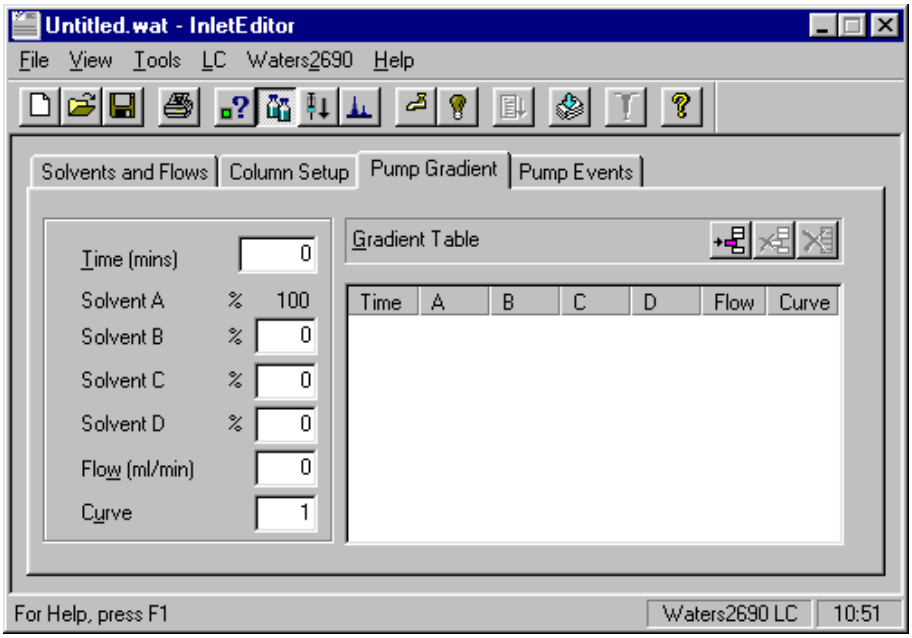


Figure 2.9 *Pump Gradient page*

This page allows a gradient to be entered and edited. If you wish to operate in isocratic mode then you should enter parameters on the Solvents and Flows page and ensure that the timetable is empty.

Time (mins) Specifies the time at which the specified conditions (%A to %D, Flow, and Curve) for the row should take effect. Make sure you set Time for the first row to 0.00, to establish initial conditions for the gradient run. The range for rows other than row 1: 0.01 to 999.99 minutes.

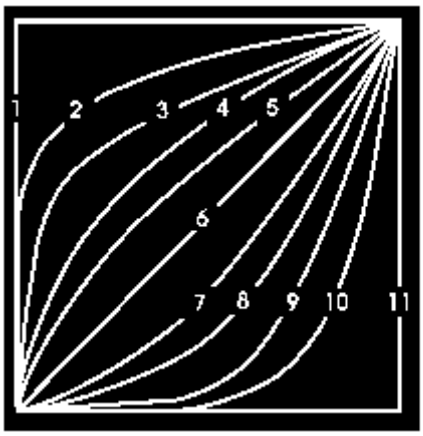
Solvent A %–Solvent D% Specifies the percentage of solvent flow from each reservoir. For each row, the total of all solvents must equal 100%. Range: 0 to 100%.

Flow (ml/min) Specifies the total flow rate for the solvent delivery system. Range: 1 to 10 ml/min.

Curve This sets the rate at which the solvent is to change to the new proportions and/or flow rates. Curves are specified by number. Available choices: 1 to 11.

Curve Number	Effect
1	Immediately goes to specified conditions
2 to 5	Convex
6	Linear
7 to 10	Concave
11	Maintains start condition until next step

Curve Profiles



- **Waters 2690 Gradient Table Operation**

To add a gradient, enter values in the relevant boxes and press the  toolbar button. You can add up to 15 rows to the table. **Note**: The first entry must have a time of 0.

To delete a single gradient, click with left mouse button on a time in the list and press the  toolbar button.

To delete all entries press the  toolbar button. This button is only available when there are entries in the timetable.

To modify a gradient, select the required entry in the timetable. The values will then be displayed in the edit boxes above the timetable, and can be altered as appropriate. Once changed press  to re-enter the values into the timetable. If, however, you modify the time value such that it does not correspond to any existing entry in the timetable pressing  will result in a new entry being created in the timetable.

Waters 2690 Pump Events Page

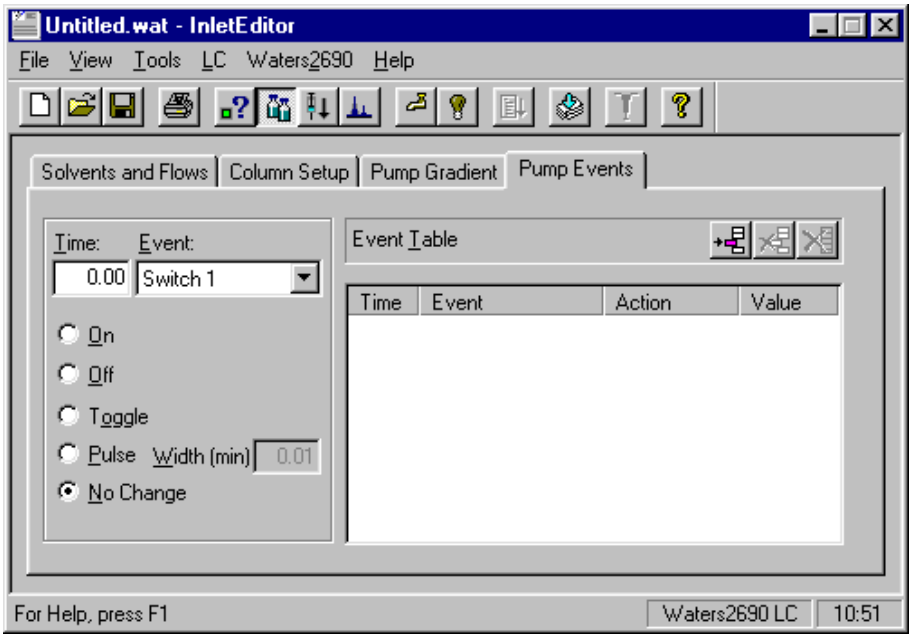


Figure 2.10 *Pump Events page*

This page allows pump events to be entered and edited.

Use the Event Table to program up to 16 events (both external and internal). The external events are triggered by four contact closures (relays) through output terminals (S1–S4) on the 2690 Separations Module. The internal events are used to control the sample compartment temperature and column heater temperature, and to prime and flush the 2690 Separations Module. Events can be triggered more than once and multiple events can be triggered simultaneously.

Time Enter the time at which the event should start. Event rows are sorted automatically by time. **Note:** Different events can be programmed to occur at the same time. Range: 0.00 to 999.99 min.

Event Enter the type of event signal required: one of the four TTL-level output switches (S1–S4), or one of the internal events (column heater temperature, sample compartment temperature or flush/prime). Available choices:

- **Switch 1** to **Switch 4** Corresponds to terminal strip positions S1 to S4 on the rear of the 2690 module. Activating a Switch event triggers a contact closure for controlling an external device. After selecting a switch event, set a state for the switch by selecting On, Off, Toggle, Pulse Width or No Change. This state appears in the Action column of the table (refer to Switch States, below). **Note:** If Pulse is selected for a switch state, the duration of the pulse must be entered in the **Width (min)** field.

- **Set Temperature (Column** or **Sample)** Specifies the temperature of an optional column heater, or an optional sample compartment heater/cooler. After selecting this event, select **Column** or **Sample** and enter the required **Temperature** in °C. **Note:** When a Column Temperature event occurs, the temperature of the column heater changes from the value set in the Heaters and Pressures page to the value set for the event. When the event times out, the temperature changes back to the Heaters and Pressures page value. Column range: 20 to 60 °C. Sample range: 4 to 40 °C.

- **Flush/Prime** Specifies a flush/prime operation for the 2690 module. Use this event only when creating Inlet Pre-run and Inlet Post-run methods. These methods will use the solvent percentages and the run time from the Solvents and Flows page but will use the **Flow** value entered on this page. **Note:** The Time field is not accessible when you select a Flush/Prime event.

Switch States

- **On** – Turns on a contact closure that triggers an external or internal event. With this function, the contact closure remains closed until an Off function is sent.
- **Off** – Turns off the contact closure for the event. With this function, the contact closure is broken.
- **Pulse** – Transmits a single On/Off pulse. The contact closure is maintained for the number of seconds defined in the Value column. Range: 0.01 to 10.00 sec.
- **Toggle** – Changes the current state of the switch.
- **No Change** – Leaves the switch in its current state.

Waters 2690 Event Table Operation

To add an event, enter a time, select an event from the drop down list box, select an action and press the  toolbar button. Up to 16 events can be programmed.

To delete a single event, click with left mouse button on a time in the list and press the  toolbar button.

To delete all entries press the  toolbar button. This button is only available when there are entries in the timetable.

To modify an event, select the required entry in the timetable. The values will then be displayed in the edit boxes above the timetable, and can be altered as appropriate. Once changed press  to re-enter the values into the timetable. If, however, you modify the time value such that it does not correspond to any existing entry in the timetable pressing  will result in a new entry being created in the timetable.

Waters 996 PDA Detector

This page is used to set parameters specific to the UV detector, to access it select **Waters996 PDA Detector** from the **View** menu or press the  toolbar button.

- **Waters 996 PDA Page**

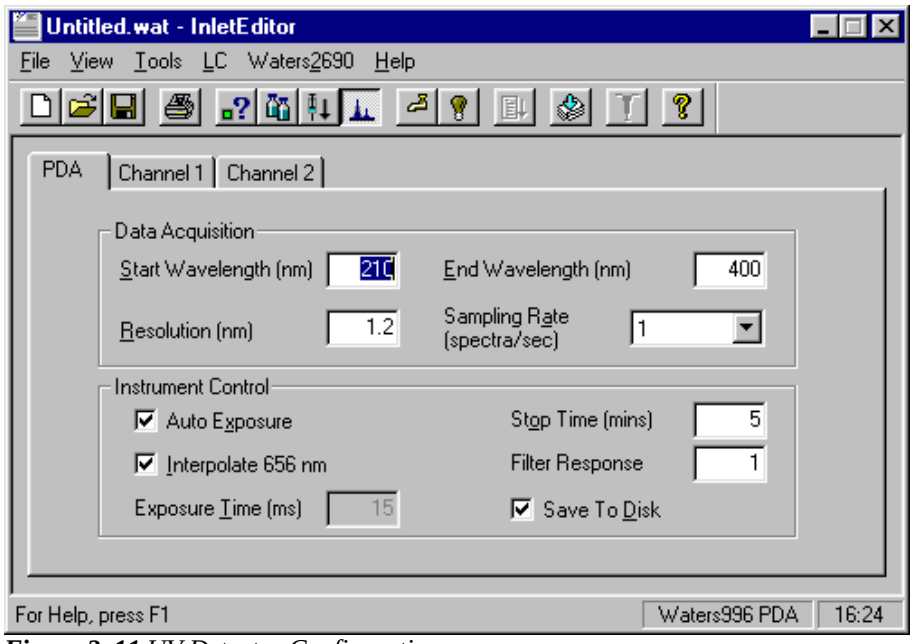


Figure 2. 11 *UV Detector Configuration page*

Start Wavelength Enter the wavelength at which to start acquiring data.

End Wavelength Enter the wavelength at which to stop acquiring data.

The range with Resolution set to 1.2 is 190.0 nm to 800.0 nm. The range at all other Resolution settings is 190.0 + (Resolution/2) to 800.0 (Resolution/2).

Resolution Enter the number of diodes that are averaged together as a single spectral data point. To differentiate closely related spectra and obtain greater spectral resolution, use a small resolution number. Be aware, however, that a small resolution value generates more data points and therefore requires more disk space than a large resolution value. Find a resolution value just small enough to identify spectral features. Range: 1.2 to 24.0 nm in multiples of 1.2.

Sampling Rate Select the number of Spectra to be acquired per second, from the dropdown list box. For good integration and quantitation, acquire 15 to 20 spectra across a peak.

Auto Exposure Check this box to enable the detector optics to calculate the optimum exposure time needed to recharge the diodes, based on the lamp energy, the lamp spectrum and the selected wavelength range. **Tip:** Enable Auto Exposure for most routine analyses.

Interpolate Check this box to instruct the detector to ignore the signal from the photodiode at 656 nm and interpolate a value from the adjacent diodes. This prevents over-saturation at 656 nm (Balmer line for deuterium). Only applicable if the **Auto Exposure** option has been selected.

If this box is not checked the detector reports the signal from the photodiode at 656 nm, this is only necessary if you are working with compounds that absorb in the 656 nm range.

Note: If this parameter is unchecked, the deuterium lamp high emission line at 656 nm may cause spectral artifacts and autoexposure errors.

Exposure Time The exposure time is the time that the photodiodes are exposed to light before they are read. To set a different Exposure Time, ensure that the Auto Exposure box is not checked and enter the required time in milli seconds.
Range: 11.00 to 500.00 ms.

Stop Time To specify a different Acquisition Stop Time enter the time in minutes when the PDA should stop scanning.

Filter Response Enter the response time for filtering acquired data. The filter is an enhanced rolling average filter applied to absorbance data from the PDA detector before the data is sent to MassLynx. The filter reduces high-frequency noise across the entire wavelength range specified for the acquisition. High values decrease peak response. Available choices: 0, 1, 2 and 3.

Save to Disk Check this box to save the Photo Diode Array data to the raw datafile. If this data is not required for further processing then uncheck the box, the data is not saved to disk thus reducing the size of the file.

■ Waters 996 Channel Detector Configuration Pages

The Channel 1 and Channel 2 pages contain the same information. Select the page relevant to the channel required, by clicking on the tab.

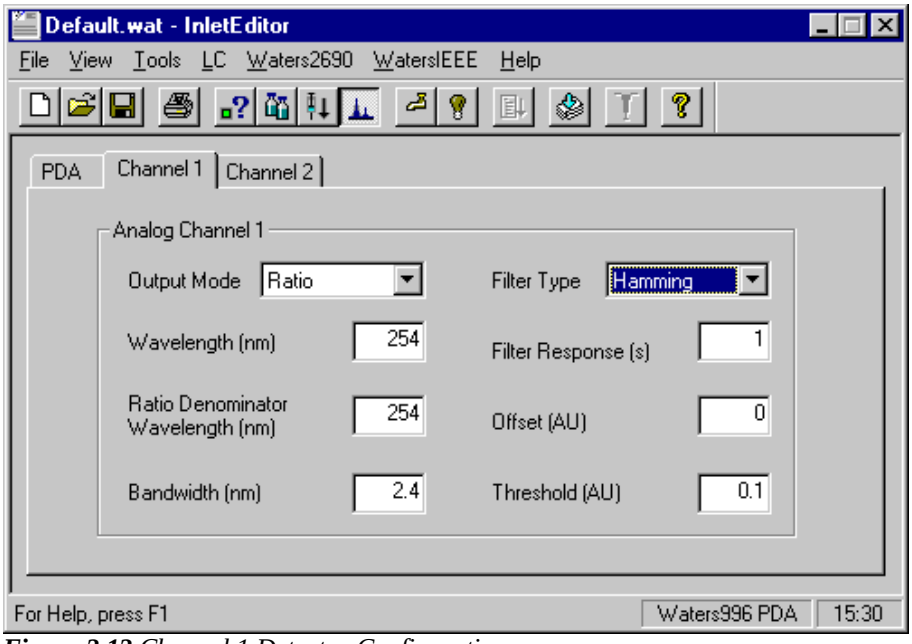


Figure 2.12 *Channel 1 Detector Configuration page*

Output Mode Select one of

- **Off –** no analog output signal.
- **Absorbance –** Output is in absorbance units at the wavelength specified. **Note: Ratio Denominator Wavelength** and **Threshold** parameters are not accessible when Absorbance mode is selected.
- **Ratio** – Output represents the ratio of absorbances at two wavelengths. The numerator wavelength is specified by the Wavelength parameter, and the denominator wavelength is specified by the Ratio Denominator Wavelength parameter (see below).

Wavelength Enter the output wavelength to monitor. In Ratio mode, the absorbance at the Wavelength is used to calculate ratio in the formula:

Ratio = Absorbance at Wavelength/Absorbance at Ratio Denominator Wavelength

Wavelength must be within the wavelength range specified by the Start Wavelength and End Wavelength parameters on the PDA page.

Range when Resolution is set to 1.2: Start Wavelength to End Wavelength.
Range at all other Resolution settings: Start Wavelength + (Bandwidth/2) to End Wavelength – (Bandwidth/2). Default: 254 nm.

Ratio Denominator Wavelength Enter the denominator wavelength (in nanometers) for the analog output channel. Ratio Denominator Wavelength must be within the wavelength range specified by the Start Wavelength and End Wavelength parameters on the 996 PDA page.

Bandwidth Enter the spectral bandwidth of the analog output channel. The range is 1.2 to 24.0 nm.

Filter Type Select **Hamming** or **Single Pole** from the dropdown list box. The Hamming filter is designed to create the same degree of peak-height degradation as the Single Pole filter for the same response time, but enhances filtering of high-frequency noise.

Filter Response Enter the response time for the filter. The range is 0 to 5 seconds.

Offset If required enter an offset to the analog output channel. The range is –0.2 to 2.0 AU.

Threshold Enter a threshold above which the ratio (Wavelength / Ratio Denominator Wavelength) must be to be valid data. The range is –0.1 to 2.0 AU.

Note: If no ratio is plotted one or both channels are below the current Threshold and a lower Threshold value should be entered.

Waters 486 UV Detector

This page is used to set parameters specific to the UV detector, to access it select **Waters486 UV Detector** from the **View** menu or press the  toolbar button.

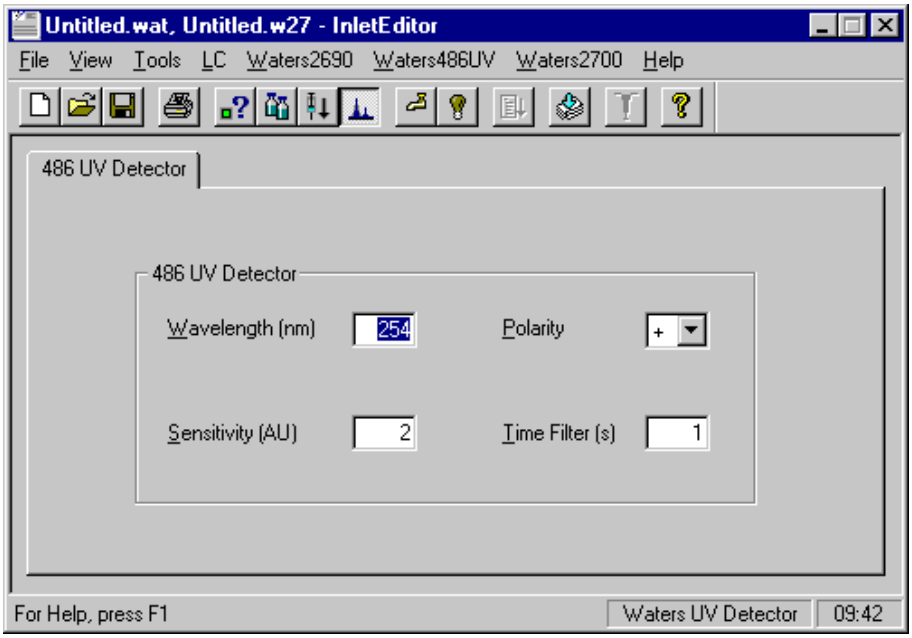


Figure 2.13 *486 UV Detector Configuration page*

Wavelength (μ) Enter the wavelength to monitor.

Polarity Select the polarity of the output signal from the drop down list box.

Sensitivity (AUFS) Enter the required sensitivity of the output signal.

Time Filter (seconds) Enter the response time for filtering acquired data.

A full description of all the parameters in this editor is given in the *Waters 486 Instruction Manual.*

Waters 2487 UV Detector

This page is used to set parameters specific to the Waters 2487 UV detector, to access it select **Waters2487 UV Detector** from the **View** menu or press the  toolbar button.

2487 Single Wavelength Absorbance Detector

The 2487 detector can be used as a single or dual wavelength detector. To use as a single wavelength detector select **Single Wavelength** from the **Waters2487UV** menu. A tick mark will appear next to the name if single wavelength is selected and the **2487 Channel B** parameters are greyed out.

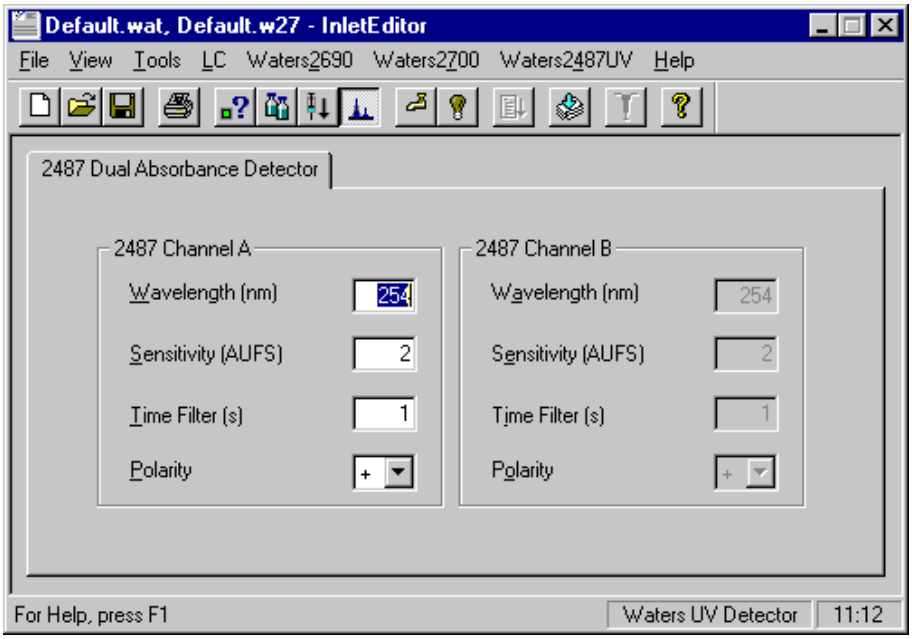


Figure 2.14 *2487 UV Detector Configuration page (Single Wavelength)*

Wavelength (μ) Enter the wavelength to monitor.

Sensitivity (AUFS) Enter the required sensitivity of the output signal.

Time Filter (seconds) Enter the response time for filtering acquired data.

Polarity Select the polarity of the output signal from the drop down list box.

A full description of all the parameters in this editor is given in the *Waters 2487 Instruction Manual.*

2487 Dual Wavelength Absorbance Detector

The 2487 detector can be used as a single or dual wavelength detector. To use as a dual wavelength detector ensure that the **Single Wavelength** option on the **Waters2487UV** menu is not selected. If a tick mark appears next to the name then single wavelength is selected, selecting the option again will return the detector to dual wavelength mode and both channel parameters will be available.

The parameters are the same as for single wavelength mode.

Waters 2487 IEEE Detector

The 2487 IEEE Detector should be selected if the detector is connected via a GPIB card in the back of the PC.

The 2487 IEEE Detector is used to collect binary data, through the IEEE interface, rather than through the analog interface.

This page is used to set parameters specific to the Waters 2487 IEEE detector, to access it select **Waters2487 IEEE Detector** from the **View** menu or press the  toolbar button.

2487 Dual Absorbance Detector

The 2487 detector can be used as a single or dual wavelength detector. To use as a single wavelength detector select **Single Wavelength** from the **Waters2487UV** menu. A tick mark will appear next to the name if single wavelength is selected and the **2487 Channel B** parameters are greyed out.

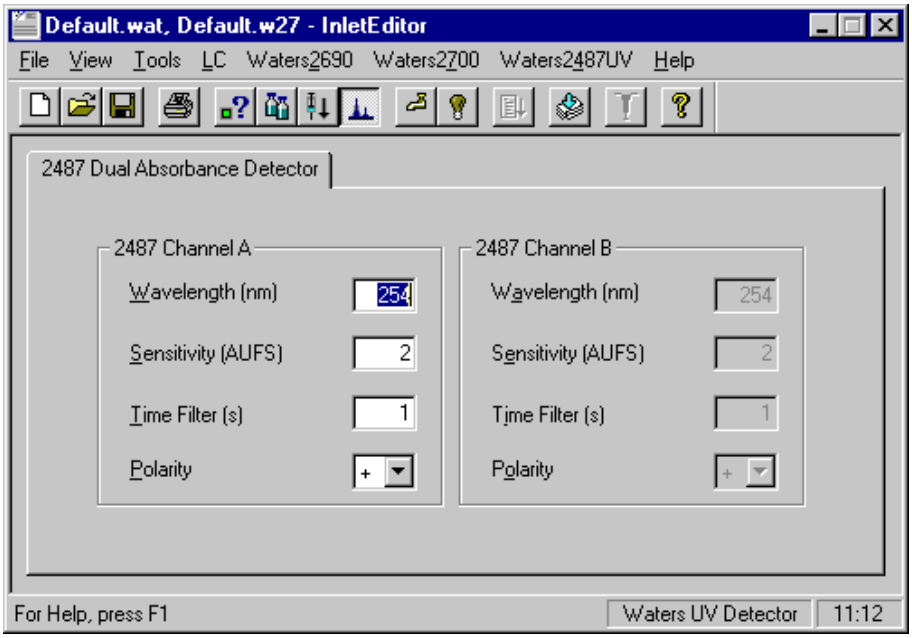


Figure 2.15 *2487 UV Detector Configuration page (Single Wavelength)*

Wavelength (μ) Enter the wavelength to monitor.

Sensitivity (AUFS) Enter the required sensitivity of the output signal.

Time Filter (seconds) Enter the response time for filtering acquired data.

Polarity Select the polarity of the output signal from the drop down list box.

A full description of all the parameters in this editor is given in the *Waters 2487 Instruction Manual.*

Waters SAT/IN PDA Detector

This page is used to set parameters specific to the PDA detector, to access it select **WatersSATIN PDA Detector** from the **View** menu or press the  toolbar button.

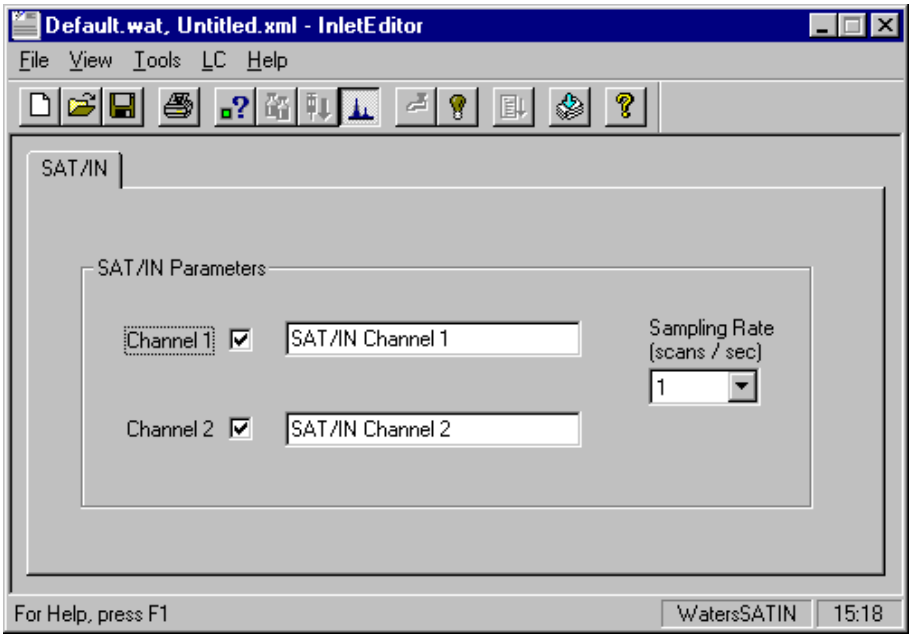


Figure 2.16 *SAT/IN Configuration page*

Channel 1 and Channel 2 Check the box(es) for the required channels.

Sampling Rate Select the number of Spectra to be acquired per second, from the dropdown list box. For good integration and quantitation, acquire 15 to 20 spectra across a peak.

Notes

Data collected through a Waters SAT/IN PDA Detector is shown as analog data in the acquired data files, this is the same as analog data coming in through the analog inputs from the back of an MS instrument.

The Waters SAT/IN PDA Detector can be used to collect analog data or the MS analog inputs can be used. Do not try to collect analog data with the SAT/IN and the MS analog inputs at the same time. Collecting analog data from both sources will result in unpredictable behaviour.

SAT/IN analog data will only be collected in a system configured with a spectral data source. An MS detector and/or a PDA detector must also be used to successfully collect SAT/IN data.

Negative data is not supported by the Waters SAT/IN but can be avoided by applying an appropriate offset in the connected Detector.

Waters 2700 Autosampler

These pages are used to set parameters specific to the autosampler, to access them select **Waters2700 AutoSampler** from the **View** menu or press the  toolbar button.

- **Waters 2700 Injection Configuration**

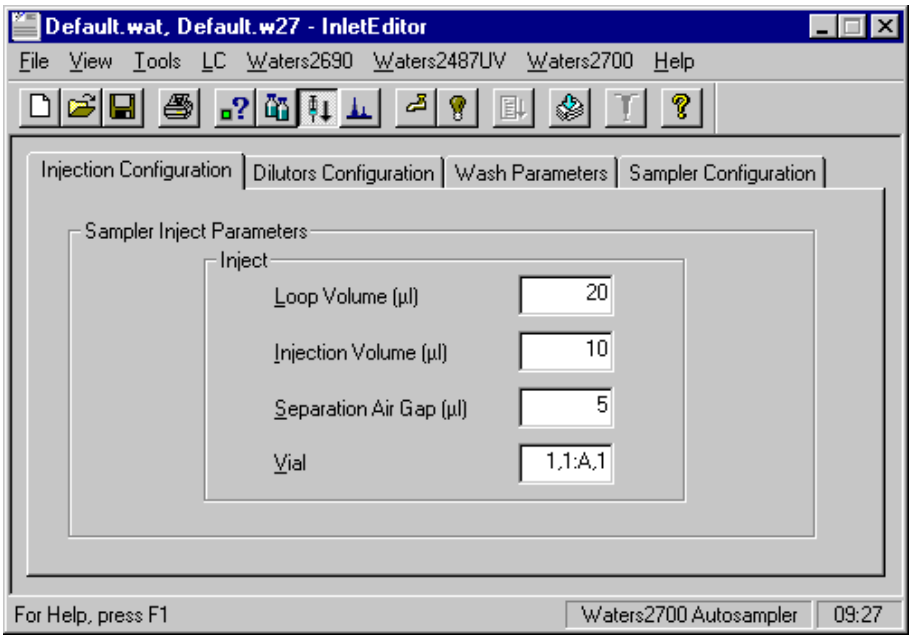


Figure 2.17 *Waters 2700 Sampler Injection Configuration Page*

Loop Volume (µl) Enter the volume of the sample loop in microlitres.

Injection Volume (µl) Enter the volume of the sample to inject into the loop for single sample acquisitions. For samples acquired via a sample list this is overridden by the value in the sample list. If the Injection Volume is equal to the Loop Volume then twice the Injection Volume is drawn to ensure that the loop is full.

Separation Air Gap (µl) Enter the volume of air to draw before the sample.

Vial Enter the position of the vial to use for single sample acquisitions. For samples acquired via a sample list this is overridden by the value in the sample list.

- **Waters 2700 Dilutor Configuration**

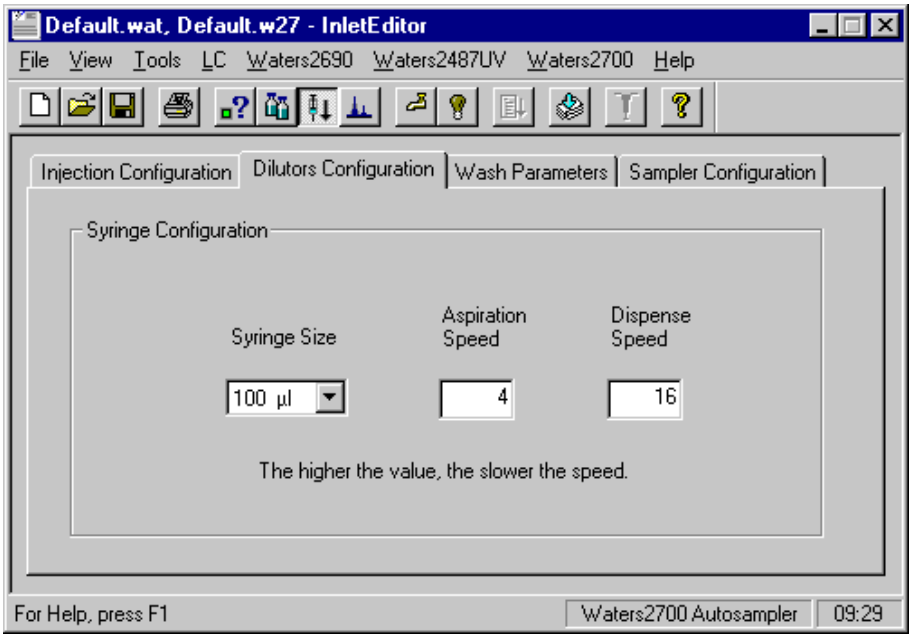


Figure 2.18 *Waters 2700 Sampler Dilutor Configuration Page*

Syringe Size Select the size of the syringe installed from the drop down list box.

Aspiration Speed Enter a value for the speed at which to draw the sample into the needle (the pump will be on its downward journey). Range: 1 to 32, with 1 being the fastest.

Dispense Speed Enter a value for the speed at which to eject the sample from the needle (the pump will be on its upward journey). Range: 1 to 32, with 1 being the fastest.

- **Waters 2700 Wash Parameters**

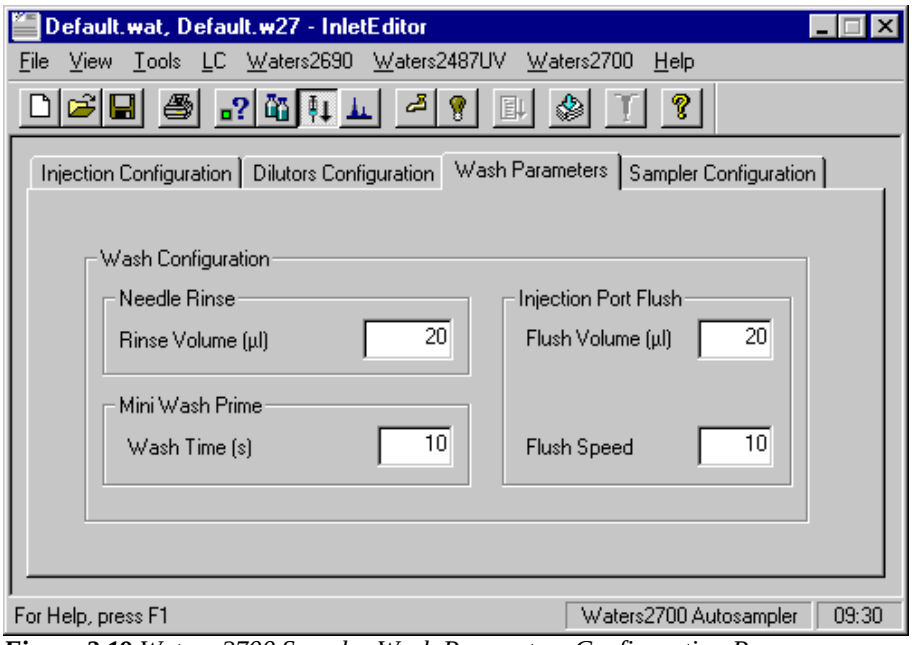


Figure 2.19 *Waters 2700 Sampler Wash Parameters Configuration Page*

Needle Rinse Volume (µl) Enter the volume of mobile phase required to wash the needle after an injection. A value of zero will result in no wash. If the needle rinse volume is greater than 800µl then the mini-wash pump is used instead.

Wash Time (seconds) Enter the time for which the mini-wash pump is activated during a mini-wash prime. Mini-wash prime is activated from the **Waters2700** menu.

Injection Port Flush Volume (µl) Enter the volume of mobile phase required to flush the inject port after the sample has been injected. A value of zero will result in no port flush.

Injection Port Flush Speed Enter the speed at which the flush volume is dispensed. Range: 1 to 32, with 1 being the fastest.

- **Waters 2700 Sample Configuration**

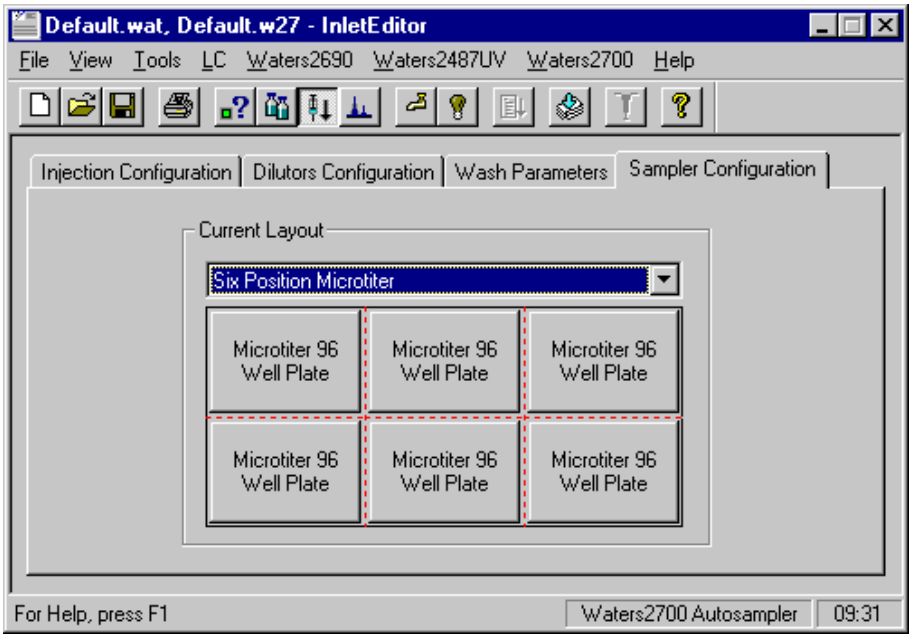


Figure 2.20 *Waters 2700 Sampler Configuration Page*

Current Layout This shows the currently selected rack configuration. To change the current layout select a new one from the drop down list box.

Waters 2700 Bed Layout

Bed layouts are created, deleted or amended from this dialog. To display the Bed Layout Editor dialog, select **Bed Layout** from the **Waters2700** menu.

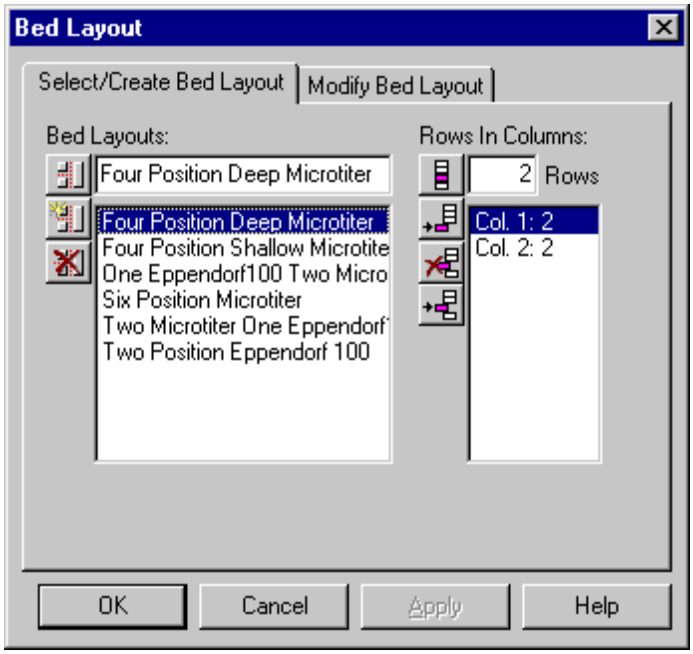


Figure 2.21 *Bed Layout Dialog*

- **To Create A New Bed Layout (Waters 2700)**

1. Highlight a bed layout similar to the one you want to create and press the  button to create a new layout. The layout appears in the **Bed Layouts** list as the same name with a 1 at the end, e.g. Six Position Microtiter1.

2. To change the name of the layout, type the new name into the Bed Layouts text box and press the  button. The name is updated in the Bed Layouts list box.

New bed layouts are saved to the MassLynx **Racks** directory.

- **To Delete A Bed Layout (Waters 2700)**

1. Highlight the bed layout to delete and press the  button. A dialog box will ask you to confirm the deletion. Press the **OK** button to delete the bed layout. **Note:** The bed layout which is selected as the current bed layout on the Sampler Configuration page cannot be deleted.

- **Other Bed Layout Options (Waters 2700)**

1. To change the number of rows in the current column, type the new number into the Rows box and press the  button.
2. To append a new column, press the  button.
3. To delete the current column press the  button.
4. To insert a column, click on the column before which you want to insert and press the  button. **Note:** The column inserted will have the same number of rows as the column highlighted.

- **Modify Bed Layout (Waters 2700)**

If the plate position or type needs changing select the **Modify Bed Layout** tab.

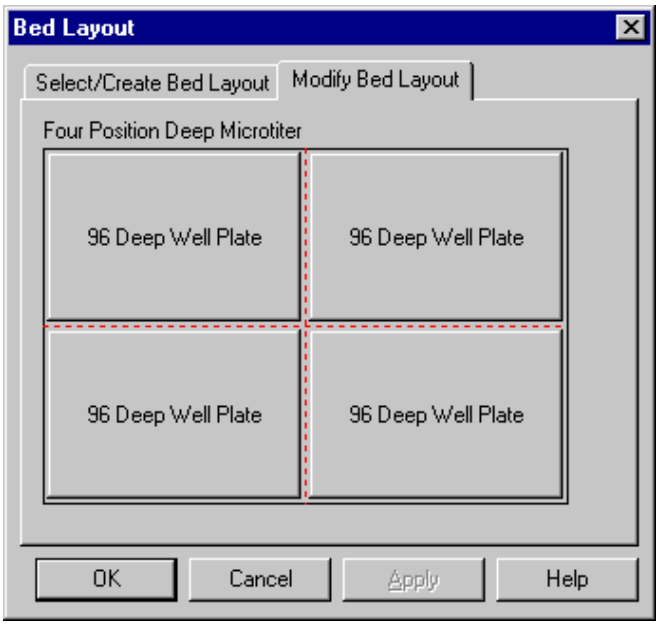


Figure 2.22 *Modify Bed Layout Dialog*

Click on one of the code plates to display the **Plate Position and Type** dialog.

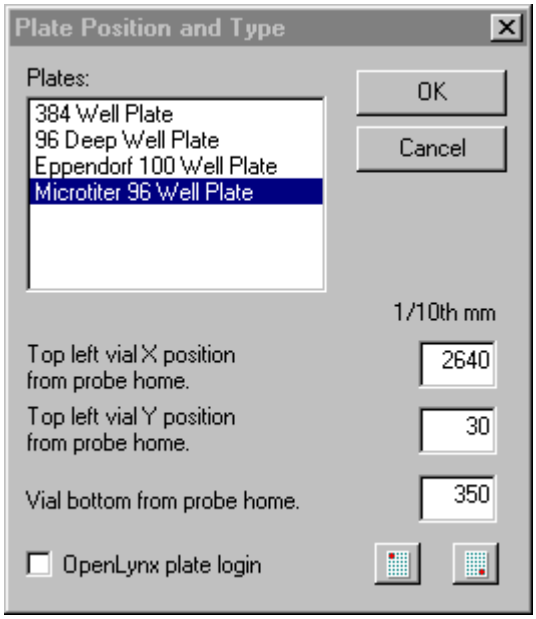


Figure 2.23 *Plate Position and Type dialog*

This dialog allows you to select a new plate from a list of possible options, and change its actual position on the bed. Measurements for plate positions are always taken from the top left corner of each plate. The **X** value is the measurement from the vial position in the top left corner of the plate to the home position. The **Y** value is the measurement from the vial position in the top left corner of the plate to the home position.

Vial bottom from probe home This is the distance the needle must travel downwards to reach the bottom of the well.

OpenLynx plate login If this box is checked and **Use current MassLynx autosampler bed layout** is checked in the OpenLynx Manager program, then the plate at this position can only be used for plate login on the OpenLynx Login program.

Pressing the  button will move the needle to the top left vial position defined by the X, Y and Vial bottom from probe home positions. If the needle is not above the top left vial then the plate will need moving or the X and Y values will need changing.

Pressing the  button will take the needle to the bottom right vial position (The software will calculate this from the plate type and the X and Y positions defined). This is used to test that the plate will fit on the autosampler, if it does not then an error message is displayed. The plate will need changing or moving or the X and Y values will need changing.

Waters 2700 Fixed Positions

This dialog allows the positions of the Injector Port, Cleaner Stations and the Waste station to be defined. It is accessed by selecting **Edit Fixed Positions** from the **Waters2700** menu.

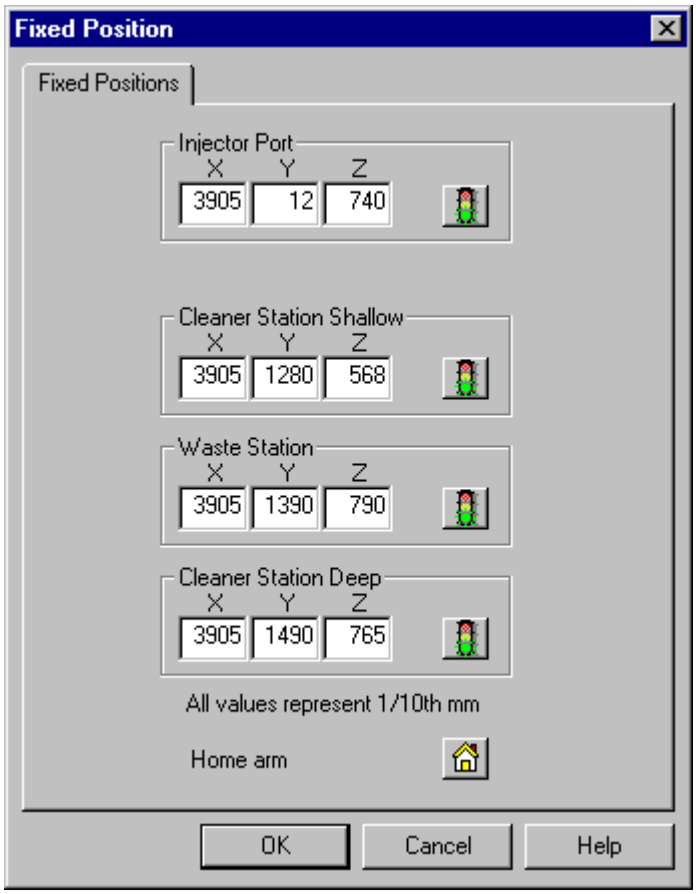


Figure 2.24 *Fixed Position Dialog*

The **X** and **Y** values are the distance the needle must travel from the Home position to the required station.

The **Z** value is the distance the needle must travel downwards to reach the required station.

To test that the values entered are valid press the  button. The needle will travel to the position specified. To return the needle to the Home position, press the  button.

When all values are correct press the **OK** button.

Waters 2700 Plate Generator

To display the Plate Generator dialog, select **Plate Generator** from the **Waters2700** menu.

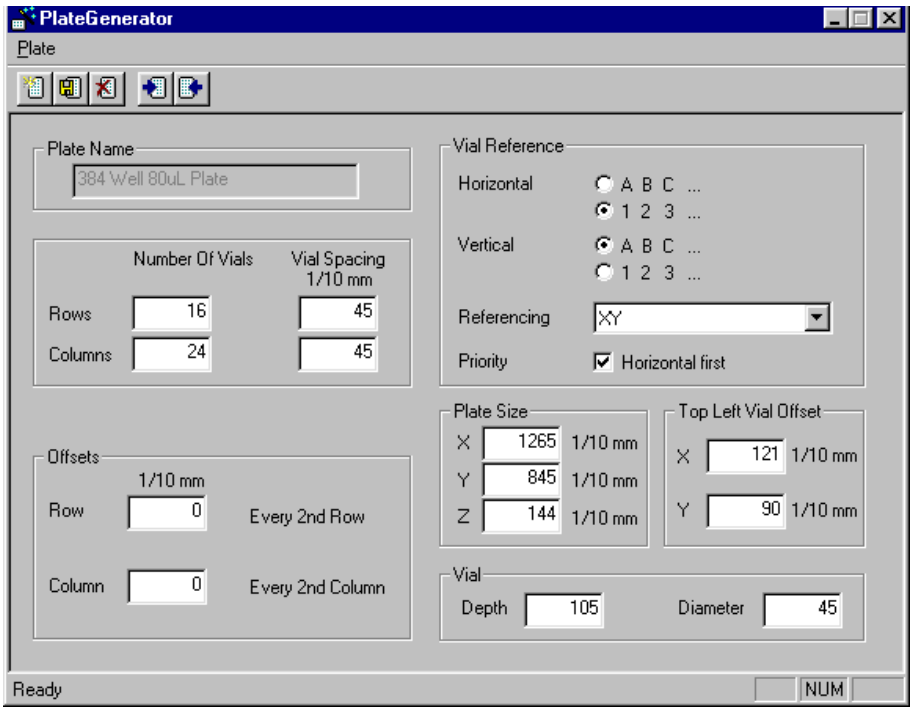


Figure 2.25 *Plate Generator*

Plate Name The name of the plate that is currently being edited.

Rows The number of vials in a row and the distance between each center.

Columns The number of vials in a column and the distance between each center.

Offsets Allows alternate vial rows or columns to be offset. **Note:** Entering a positive value will shift even numbered rows to the right and negative values will shift even numbered rows to the left.

Vial Reference Allows the user to select the way that the vial rows and columns are referenced, e.g. whether the rows are alphabetical or numerical.

Referencing This has three options

- XY which references the vials A1, B1 etc.
- Sequential Discontinuous which numbers the vials 1, 2, 3 across a row, left to right, and then starts the next row from the left again.
- Sequential Continuous which numbers the vials 1, 2, 3 across a row, left to right, then continues number the next row, right to left etc.

If the Waters 2700 autosampler is used with OpenLynx then the vial referencing must be set to either sequential continuous or sequential discontinuous.

Priority Check the **Horizontal First** box if samples are to be acquired horizontally across the plate.

If Referencing = X,Y, Horizontal = Letter, Vertical = Number and Horizontal Priority is checked, this will result in samples being acquired in the order A1, A2, A3. If the Horizontal Priority box is not checked samples will be acquired in the order 1A, 1B, 1C etc.

If Referencing = sequential continuous or discontinuous and Horizontal Priority is checked, this will result in samples being acquired from row 1 then row 2. If the Horizontal Priority box is not checked samples will be acquired from column 1 then column 2 etc.

Plate Size The size of the plate to its outside edges.

Top Left Vial Offset The measurement to the center of the first vial from the top left corner of the plate.

Vial The depth and diameter values are used for display only. They appear in the description for a single shot login on the OpenLynx Login screen.

Creating and Deleting Waters 2700 Plates

To create a new plate, press the  button. A new default plate is displayed, change the **Plate Name**, enter the appropriate values and press the save  button or select **Save Plate** from the **Plate** menu. New plates are saved to the MassLynx **Plates** directory.

To copy a plate, page through the list of saved plates using the  and  toolbar buttons. The **Previous Plate** and **Next Plate** options on the **Plate** menu perform the same operation. When the required plate is displayed change the **Plate Name**, enter the appropriate values and press the save  button or select **Save Plate** from the **Plate** menu. New plates are saved to the MassLynx **Plates** directory.

To delete a plate select the plate, by typing the name in the **Plate Name** box or by paging through as above, and press the delete  button or choose **Delete Plate** from the **Plate** menu.

Note: All of the spacings and the **vial section** are stored in 0.1mm units.

Note: When defining a custom plate for use with a multi-injector the plate is required to be compatible with the position of the 8 needles of the autosampler.

- The Plate must have eight columns.
- The position of the vials should allow all eight needles to enter a separate vial.
- There should be no odd or even offsets for any of the vial positions.

Note: If the Plate currently selected on the Sample Configuration page is changed here, then **Reset Injector** should be selected from the **LC** menu to reset communications.

Waters 2700 Menu

Prime Syringe This option is used to remove air from the syringe and any tubing connected to it. It repeatedly draws the mobile phase into the needle and flushes it out until the  toolbar button is pressed, or **Stop Method** is selected from the **LC** menu, on the Inlet Editor. **Note:** Before Prime Syringe is selected the toolbar button appears as  and the menu as **Run Method**.

Change Syringe Selecting this option moves the needle to a position where it can be removed and replaced. When the syringe has been changed, Prime Syringe should then be selected to get the needle into a state ready for injection.

Prime Mini-Wash This option moves the needle to the waste position and pumps the mobile phase through it for the **Wash Time** defined on the **Wash Parameters** page.

Waters 2790 Autosampler

Note: To control the Waters 2790 autosampler and pump from the keypad rather than the MassLynx software the **Inlet** must be configured as **None**. See Configuring the Inlet System in the Acquisition Control Panel chapter.

These pages are used to set parameters specific to the Sampler, to access them select **Waters2790 AutoSampler** from the **View** menu or press the  toolbar button.

Waters 2790 Injection Parameters Page

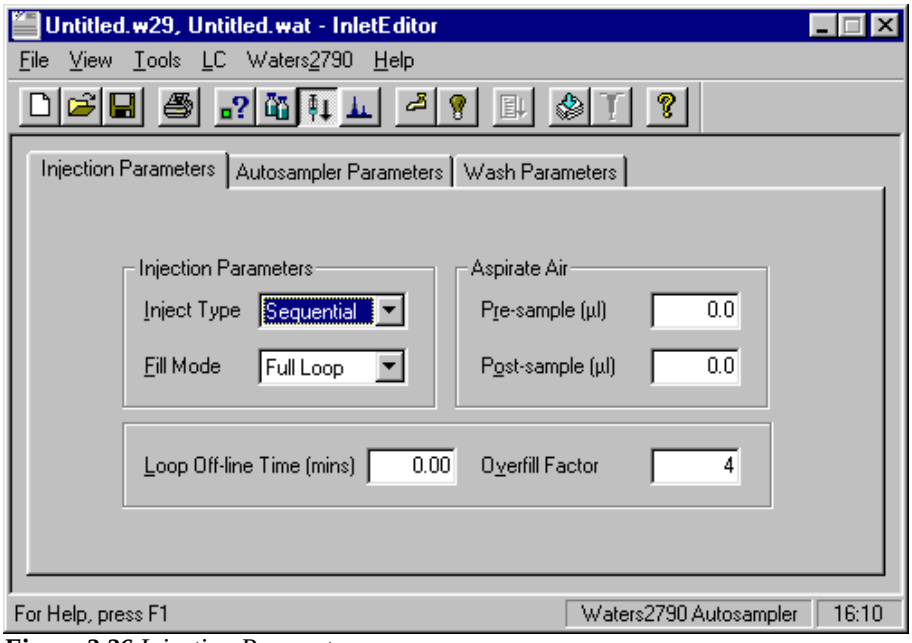


Figure 2.26 *Injection Parameters page*

Inject Type Select Sequential or Parallel from the drop down list box.

Sequential – Sample aspiration occurs at the start of each injection cycle, after completion of the previous injection.

Parallel – Sample aspiration and loop fill occur concurrently with other separation method functions for higher throughput.

Fill Mode Select Full Loop or Partial Loop from the drop down list box.

Full Loop – The autosampler draws in the loop volume the overfill factor number of times, to ensure that the loop is full.

Partial Loop – The autosampler will draw in the volume specified in the sample list and centre it in the loop.

Aspirate Air Pre-sample Enter the volume of air to be drawn into the needle before the sample, to separate it from the previous sample. Range: 0 to half the loop size.

Aspirate Air Post-sample Enter the volume of air to be drawn into the needle after the sample, to separate it from the next sample. Range: 0 to half the loop size.

Loop Off-line Time For Parallel Injection mode, enter the time in minutes when the injector valve is switched back from the inject position to the load position for the next sample to be preloaded into the sample loop. Range 0.00 to the Run Time defined on the Pump Mobile Phase page, in minutes.

Overfill Factor For full loop mode enter the number of times to draw the loop volume into the loop to ensure that it is full. Range 1.0 to 20.

- **Waters 2790 Autosampler Parameters Page**

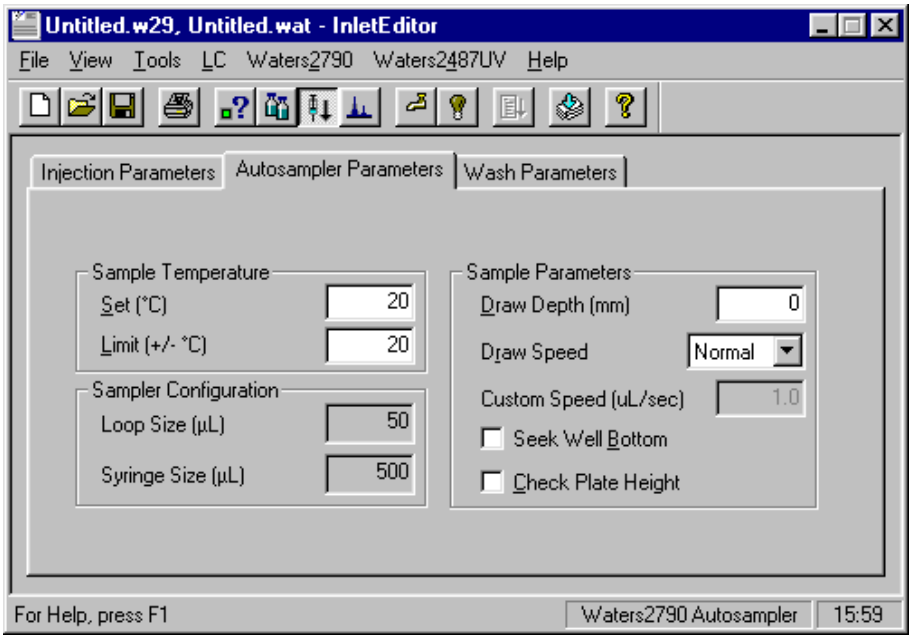


Figure 2.27 *Autosampler Parameters page*

Sample Temperature Set If the sample heater is installed, enter the temperature to heat or cool the sample to. Range: 4.0 to 40.0 °C.

Sample Temperature Limit This is the maximum deviation in sample temperature allowed. If this is exceeded the current acquisition will stop and the LC Status error light, on the MassLynx screen, will turn red. Range: ±1.0 to ±20.0 °C.

Loop Size (µl) This is a display only field showing the volume of the sample loop installed.

Syringe Size This is a display only field showing the size of the syringe installed.

Draw Depth Adjusts the depth of the needle tip to accommodate for sedimented samples or non-standard vials. A value of 0 corresponds to the bottom of the vial. Range: 0.0 to 20.0 mm.

Draw Speed This determines the rate in microlitres per second at which sample is extracted into the autosampler needle. This should be set according to the viscosity of the sample. Select one of **Fast**, **Normal** or **Slow** from the dropdown list box. The table below shows the draw rate for each selection using a 250 µl syringe.

Selection	Draw Rate for a 250 µl Syringe
Fast	5.0 µl/sec
Normal	2.5 µl/sec
Slow	1.0 µl/sec
Custom	Value entered in the Custom Speed box.

Seek Well Bottom If this box is checked then, for the first well on a plate, the needle will automatically seek the bottom of the well before drawing the sample. The depth of the well will be saved by the software and used as the depth for all other wells on the plate. This will be repeated for the first well on each plate. **Note:** If a value has been entered in the **Draw Depth** field then this operation will not be performed.

Check Plate Height If this box is checked, for the first injection from a plate, a needle positioning sensor determines the plate height then checks it against the Plate Size, Z value defined in the Plate Generator.

Waters 2790 Wash Parameters Page

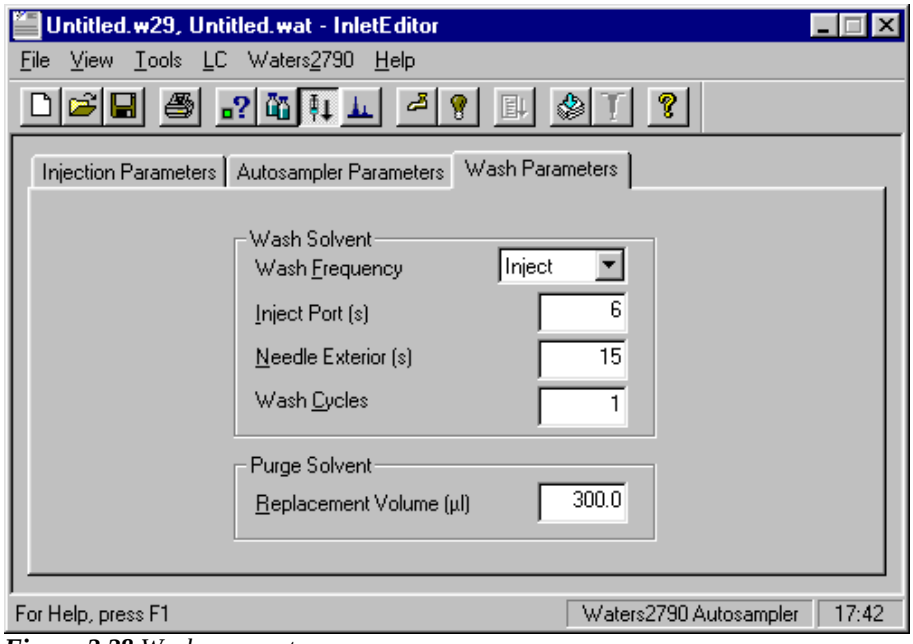


Figure 2.28 *Wash parameters page*

Wash Frequency Select the wash frequency from the drop down list box.

- **None** Do not perform a wash.
- **Inject** Perform a wash after each injection.
- **Well** Perform a wash after all samples have been taken from the current well.

Inject Port Enter the time in seconds to wash the interior of the needle for.

Needle Exterior Enter the time in seconds to wash the exterior of the needle for. Range: 0 to 99 seconds.

Wash Cycles Enter the number of times the Inject Port and Needle Exterior washes are to be performed. Range: 0 to 10.

Replacement Volume Enter the volume of wash solvent to leave in the needle after the wash/flush operation has been performed. This volume is then drawn through the waste valve and dispensed into the sample line through the needle. Range: 0 to 9999 µl.

Waters 2790 Pump

Note: To control the Waters 2790 autosampler and pump from the keypad rather than the MassLynx software the **Inlet** must be configured as **None**. See Configuring the Inlet System in the Acquisition Control Panel chapter.

The Waters Pump pages can be accessed by selecting **Waters2790 Pump** from the **View** menu on the Inlet Editor or by pressing the  toolbar button.

Waters 2790 Mobile Phase Page

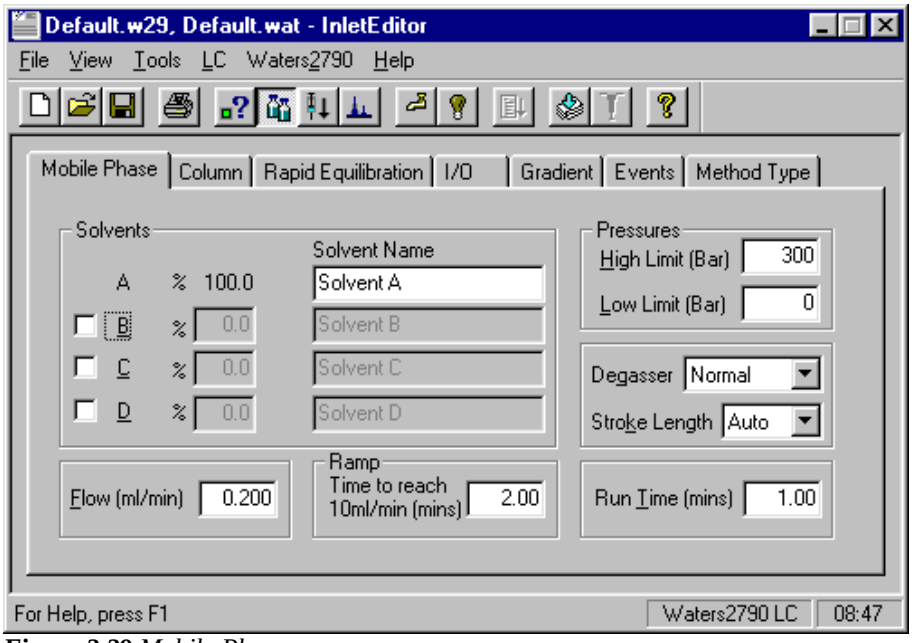


Figure 2.29 *Mobile Phase page*

Solvents Up to four solvents will be displayed depending upon the system configuration. The total value of all the solvent percentages added together must equal 100%. Solvent Names entered here will be displayed on the Gradient page.

Pump A This displays the remainder percentage after the solvent percentages have been set for the other enabled pumps.

Pump B, C and **D** These can either be enabled or disabled by checking the box next to the individual pumps. The values can be set to the required percentage of flow delivery.

Flow Enter the total initial flow rate of the system. Range: 0.000 to 10.000 ml/min.

Ramp Enter the time (in minutes) for the solvent delivery system to reach the maximum system flow rate (10 ml/min). This limits the rate of change of the flow rate to protect the column from potentially damaging sudden changes in pressure. Range: 0.01 to 30 minutes. Recommended minimum setting: 0.5 min.

Enter **Low Pressure Limit** and **High Pressure Limit** values as required. If the pressure falls outside these limits the current acquisition will stop and the LC Status error light, on the MassLynx screen, will turn red. Low Pressure Range: 0 to 310 bar. High Pressure Range: 0 to 345 bar.

Degasser Select one of **Off**, **Normal** or **Continuous** from the drop down list box.

- **Off** The degasser is always off.
- **Normal** The degasser cycles on and off.
- **Continuous** The degasser is always on.

Stroke Length This sets the volume of solvent delivered for each piston stroke. Select the required option from the drop down list box. If **Auto** is selected then the volume is automatically adjusted to provide optimal performance for the selected solvent flow rate, otherwise the volume selected will be used.

Run Time Enter the time in minutes that the method will run from the point of injection.

Note: Run time is for the solvent delivery system only. Detectors have independent run times. The MS method (Scan Function Editor) run time must be greater than all other run times.

Waters 2790 Column Page

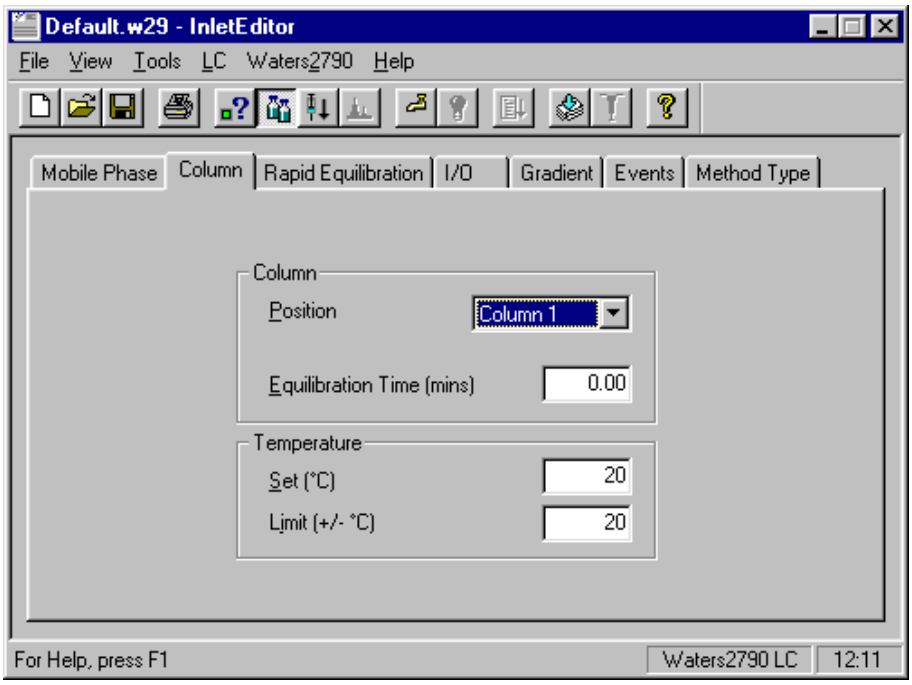


Figure 2.30 *Column page*

Position This field allows the column to be selected for the method. The options available will depend on the column setup on the Waters 2790 Separations Module.

If only one column is installed then this box will display **Column 1** and cannot be changed. For other configurations this box will allow the selection of a column (between 1 and 6 depending on configuration) or No change from the drop down list box. Selecting a numbered column will use this column for the method, selecting No Change will use the column defined in the last method used to acquire a sample. See the *Waters 2790 Separations Module Operator's Guide* for more information on the column selection valve.

Equilibrium Time Enter the time required to reach equilibrium (i.e. run in initial conditions), before performing an injection, after a column change. Range: 0.00 to 999.99 minutes.

Temperature Set Enter the target operating temperature for the optional column heater. This value must be at least 5 °C above ambient. Range: 20 to 60 °C.

Temperature Limit Enter the maximum deviation in column temperature allowed. If this is exceeded the current acquisition will stop and the LC Status error light, on the MassLynx screen, will turn red. Range: ±1 to ±20 °C.

- **Waters 2790 Rapid Equilibration Page**

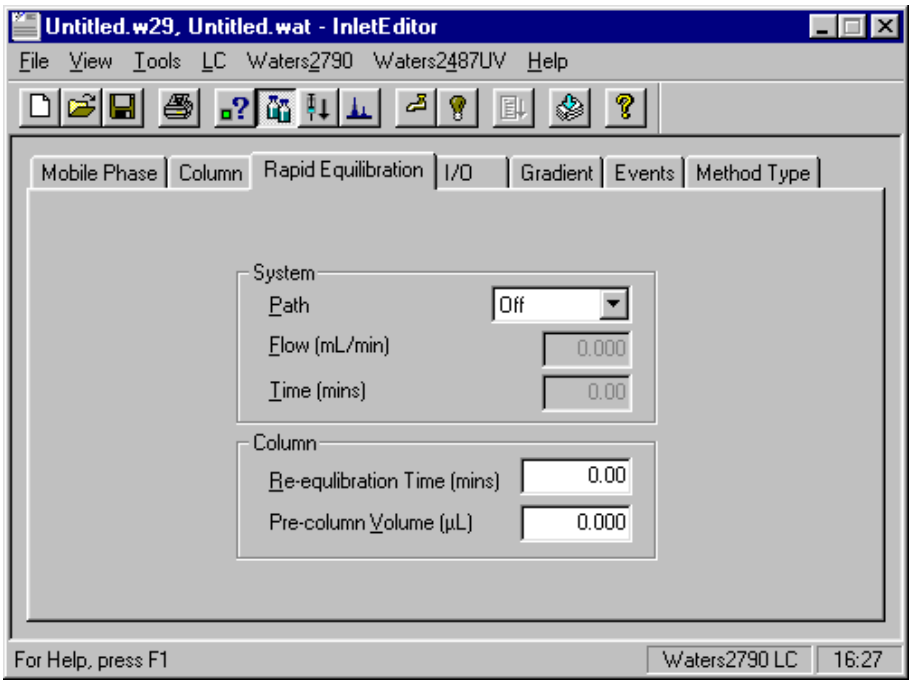


Figure 2.31 *Rapid Equilibration page*

Path Select the path to be used for flushing solvent during rapid equilibration from the drop down list box. **Waste**, **Off** or **Column 1** to **Column 6** depending on the instrument configuration.

Flow Enter the system equilibration flow rate. Range: 0.00 to 10.00 ml/min.

Time Enter the length of time (in minutes) to equilibrate. Range 0.00 to 999.99 minutes.

Re-equilibration Time Enter the time that column should be maintained at initial flow/composition conditions after completion of a gradient run. This delay is imposed on a per injection basis if defined.

Pre-column Volume Enter the volume of solvent to pump through the column between the time the gradient starts and the time of injection. Range: 0.0 to 10000.0 µl.

Waters 2790 I/O Page

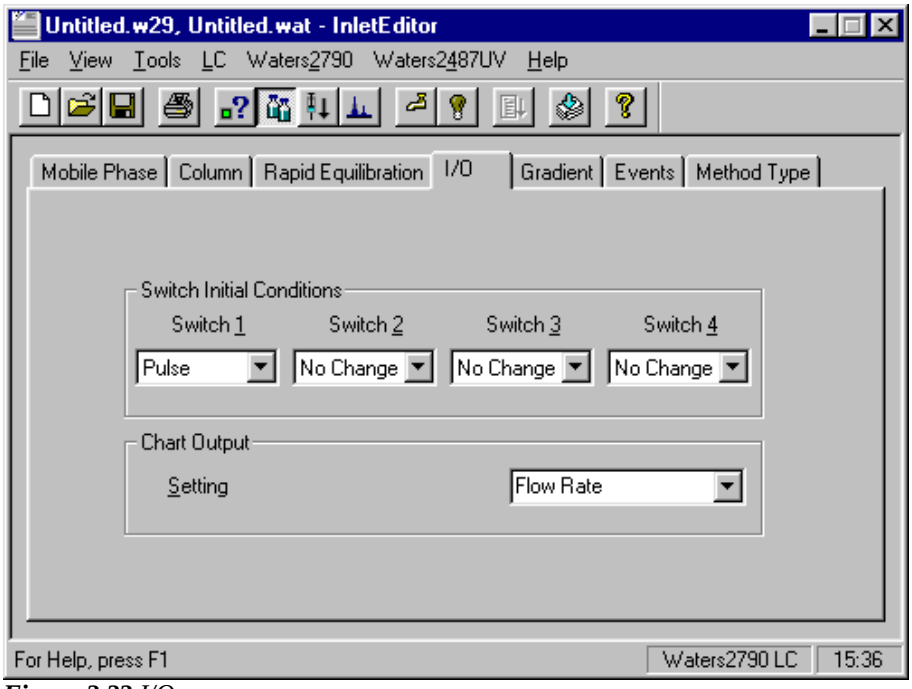


***Figure 2.32** I/O page*

Switch Initial Conditions Select the state that switches 1 to 4 should be in initially, from the drop down list box. At the beginning of each injection cycle each switch returns to the state defined here. Available choices:

- **On** – Turns on a contact closure that triggers an external or internal event. With this function, the contact closure remains closed until an Off function is sent.
- **Off** – Turns off the contact closure for the event. With this function, the contact closure is broken.
- **Pulse** – Transmits a single On/Off pulse. The contact closure is maintained for the number of minutes set in the Pulse Width field on the Events page. Range: 0.01 to 100.00 sec.
- **Toggle** – Changes the current state of the switch.
- **No Change** – Leaves the switch in its current state.

Chart Output Setting Select **Flow Rate**, **System Pressure**, **%A**, **%B**, **%C**, **%D**, **Column Temperature** or **Sample Temperature** from the drop down list box.

The Analog output signals are sent through the terminals on the back of the 2790, to an optional analog device such as a strip chart recorder. If, for example, System Pressure is selected the recorder will chart the system pressure while the method is being run.

- **Waters 2790 Gradient Page**

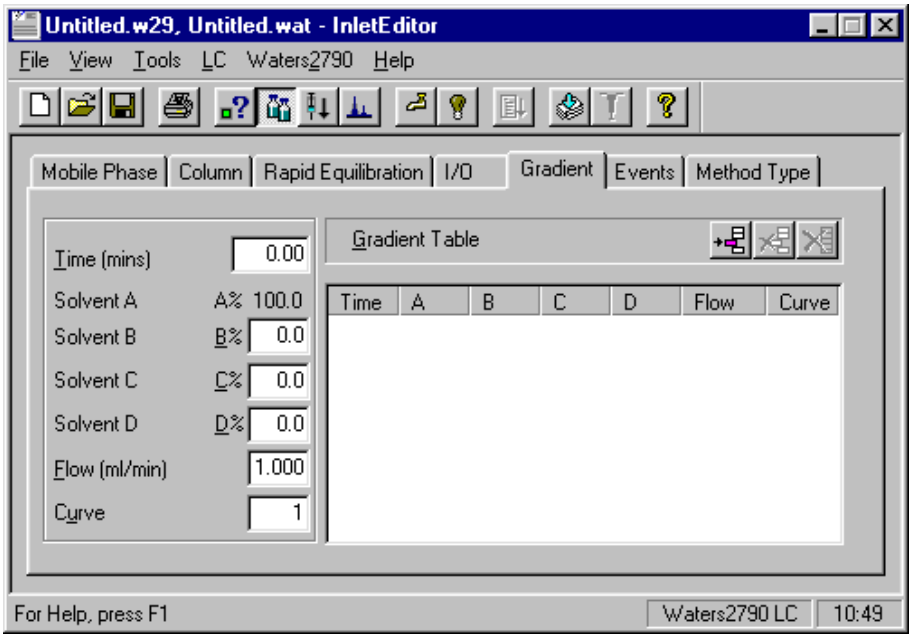


Figure 2.33 *Gradient page*

This page allows a gradient to be entered and edited. If you wish to operate in isocratic mode then enter parameters on the Mobile Phase page and ensure that the timetable is empty.

Time (mins) Specifies the time at which the specified conditions (%A to %D, Flow, and Curve) for the row should take effect. Make sure the Time for the first row is set to 0.00, to establish initial conditions for the gradient run. The range for rows other than row 1is 0.01 to 999.99 minutes.

Solvent A % - Solvent D% Specifies the percentage of solvent flow from each reservoir. For each row the total of all solvents must equal 100%. Range: 0 to 100%.

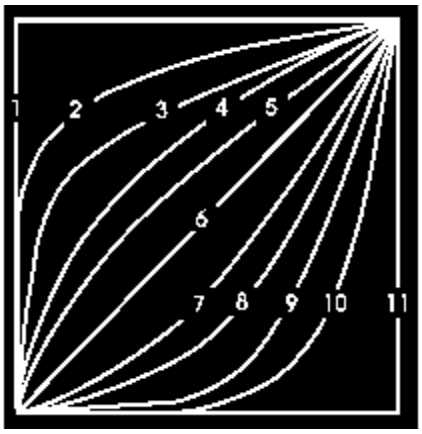
Flow (ml/min) Specifies the total flow rate for the solvent delivery system. Range: 1 to 10 ml/min.

Note: If column equilibration, rapid equilibration or wet prime are performed then the flow rate will return to the value defined on the Mobile Phase page. If they are not performed then the flow rate will stay at the value defined for the last entry in the Gradient Table. To return to the initial flow rate an entry must be added to the end of the table setting the value to that defined on the Mobile Phase page.

Curve This sets the rate at which the solvent is to change to the new proportions and/or flow rates. Curves are specified by number. Available choices: 1 to 11.

Curve Number	Effect
1	Immediately goes to specified conditions
2 to 5	Convex
6	Linear
7 to 10	Concave
11	Maintains start condition until next step

Curve Profiles



Waters 2790 Gradient Table Operation

To add a gradient, enter values in the relevant boxes and press the  toolbar button. Up to 15 rows can be added to the table. **Note:** The first entry must have a time of 0.

To delete a single gradient click with left mouse button on a time in the list and press the  toolbar button.

To delete all entries press the  toolbar button. This button is only available when there are entries in the timetable.

To modify a gradient, select the required entry in the timetable. The values will then be displayed in the edit boxes and can be altered as appropriate. Once changed press  to re-enter the values into the timetable. If, however, you modify the time value such that it does not correspond to any existing entry in the timetable pressing  will result in a new entry being created in the timetable.

Waters 2790 Events Page

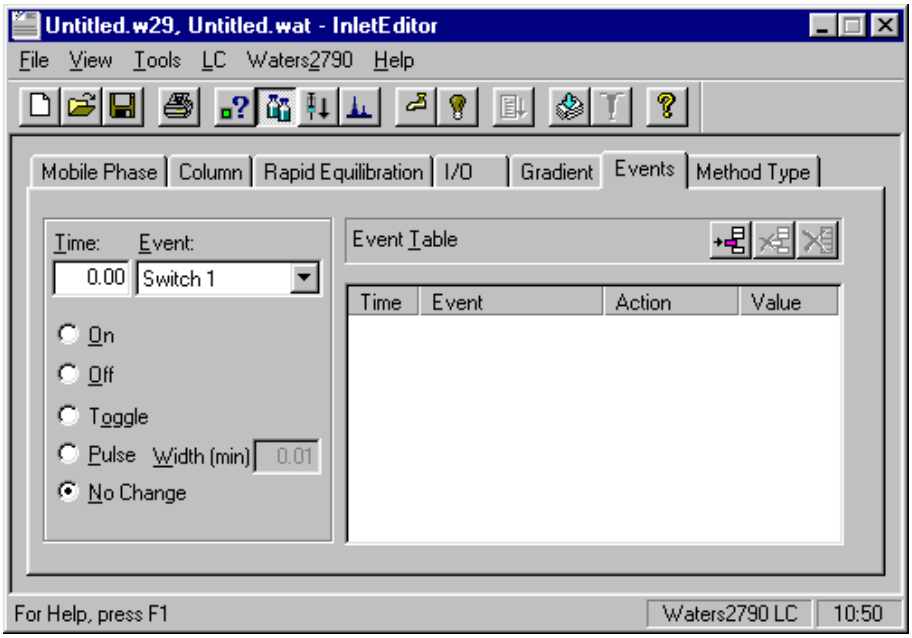


Figure 2.34 *Events page*

Use the Event Table to program up to 16 events (both external and internal). The external events are triggered by four contact closures (relays) through output terminals (S1–S4) on the 2790 Separations Module. The internal events are used to control the sample compartment temperature, column heater temperature and column change. Events can be triggered more than once and multiple events can be triggered simultaneously.

Time Enter the time at which the event starts. Event rows are sorted automatically by time. **Note:** Different events can be programmed to occur at the same time. Range 0.00 to the Run Time defined on the Mobile Phase page, in minutes.

Event Enter the type of event signal: one of the four TTL-level output switches (S1-S4), or one of the internal events (column heater temperature, sample compartment or column change).

- **Switch 1** to **Switch 4** Corresponds to terminal strip positions S1 to S4 on the rear of the 2790 module. Activating a Switch event triggers a contact closure for controlling an external device. After selecting a switch event, set a state for the switch by selecting On, Off, Toggle, Pulse Width or No Change. This state appears in the Action column of the table (see Switch States, below). **Note:** If Pulse is selected the duration of the pulse must be entered in the Width (min) field.

- **Set Temperature (Column** or **Sample)** Specifies the temperature of an optional column heater, or an optional sample compartment heater/cooler. After selecting this event, select **Column** or **Sample** and enter the required **Temperature** in °C. **Note:** When a Column Temperature event occurs, the temperature of the column heater changes from the value set in the Column page to the value set for the event. When the event times out, the temperature changes back to the Column page value. Column range: 20 to 60 °C. Sample range: 4 to 40 °C.

- **Column Change** Specifies a column change operation for the 2790 module, as describe on the Column page.

Switch States

- **On** – Turns on a contact closure that triggers an external or internal event. With this function, the contact closure remains closed until an Off function is sent.
- **Off** – Turns off the contact closure for the event. With this function, the contact closure is broken.
- **Toggle** – Changes the current state of the switch.
- **Pulse** – Transmits a single On/Off pulse. The contact closure is maintained for the number of seconds that defined in the Value column. Range: 0.01 to 10.00 sec.
- **No Change** – Leaves the switch in its current state.

Waters 2790 Event Table Operation

To add an event, type in a time, select an event from the drop down list box, select an action and press the  toolbar button. Up to 16 events can be programmed.

To delete a single event click with left mouse button on a time in the list and press the  toolbar button.

To delete all entries press the  toolbar button. This button is only available when there are entries in the timetable.

To modify an event select the required entry in the timetable. The values will then be displayed in the edit boxes and can be altered as appropriate. Once changed press  to re-enter the values into the timetable. If, however, you modify the time value such that it does not correspond to any existing entry in the timetable pressing  will result in a new entry being created in the timetable.

Waters 2790 Method Type Page

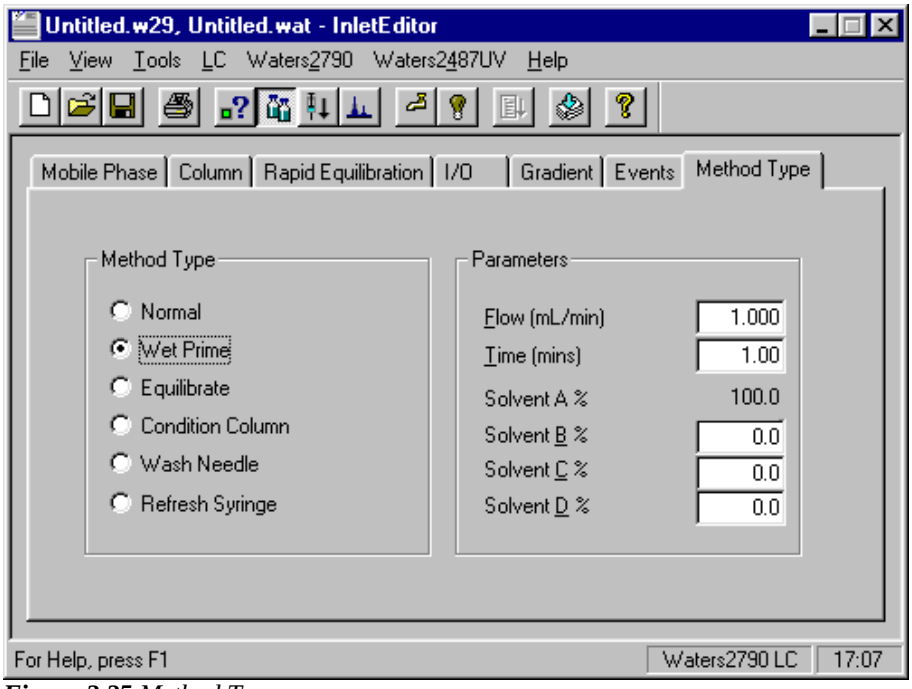


Figure 2.35 *Method Type page*

This page is used for creating normal, pre and post run methods. First create a **Normal** method and save the file, then create any pre or post run methods (saving them under different names). These methods can then be defined in the Inlet Prerun and Inlet Postrun columns of the Sample List.

Method Type Select the type of method to create. The **Parameters** section will be updated to show the parameters required for the selected method.

Normal Creates a normal method. No extra parameters need to be defined.

For all other method types see the Waters 2790 Menu, on page 53 for details of the parameters required.

Waters 2790 Menu

Waters 2790 Wet Prime

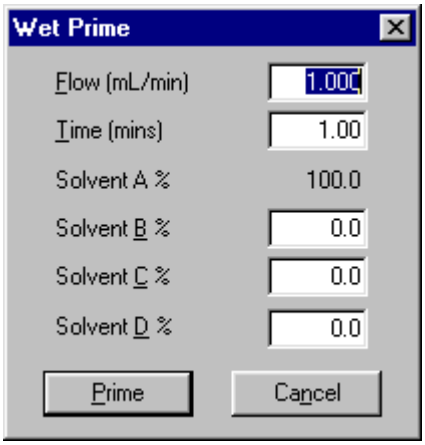


Figure 2.36 *Wet Prime dialog*

Wet Prime A wet prime should be performed when changing the solvent in the system to flush out the previous solvent. The new solvent is pumped through the tubing and the Prime port of the Inject valve to waste.

Enter the **Flow** rate, **Time** and the **Percentage of solvents** to use then press the **Prime** button. Waters recommend that the wet prime is started using the solvent with the lowest viscosity to help purge air from the lines, especially if the in-line vacuum degasser is installed.

Note: If the solvent lines are dry then a dry prime must be performed before a wet prime. See the *Waters 2790 Separation Module Operator's Guide* for more information on performing a dry prime.

Waters 2790 Equilibrate

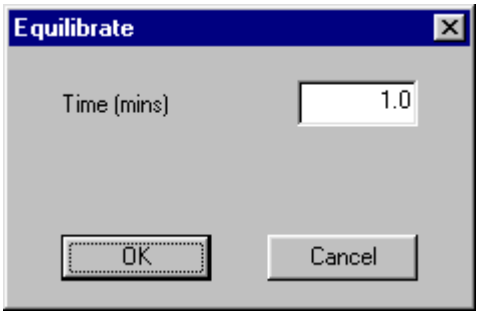


Figure 2.37 *Equilibrate dialog*

Equilibrate Equilibrates the system using the parameters defined on the Mobile Phase page.

Enter the **Time** to equilibrate the system for and press **OK**. The time needed to equilibrate the system will depend on environmental and application-specific factors.

Waters 2790 Condition Column

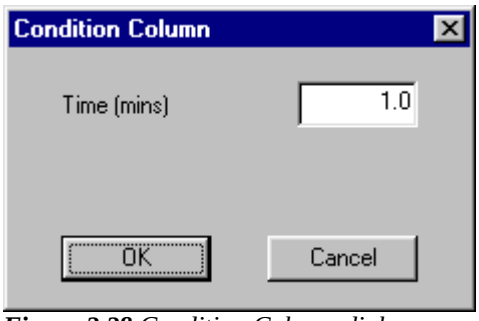


Figure 2.38 *Condition Column dialog*

Condition Column Runs solvent through the column without injecting samples or running the Events table. Solvent is delivered to the Column defined on the Column page, using the Gradient Table defined on the Gradient page.

Enter the **Time** in minutes to condition the column for and press **OK**. Ensure that the time is equal to or greater than the Time of the last entry in the Gradient Table (defined on the Gradient page) plus the Re-equilibration Time (defined on the Rapid Equilibration page).

Waters 2790 Wash Needle

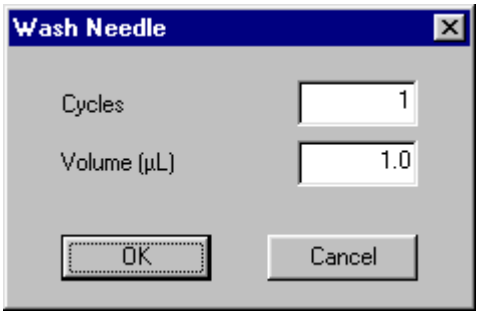


Figure 2.39 *Wash Needle dialog*

Wash Needle Washes the inject port, and both the interior and exterior of the needle with wash solvent, and then fills the needle with fresh solvent.

Enter the number of wash **Cycles** to perform and the **Volume** of wash solvent to use then press **OK**. Waters recommend a volume of 600 µl.

Waters 2790 Refresh Syringe

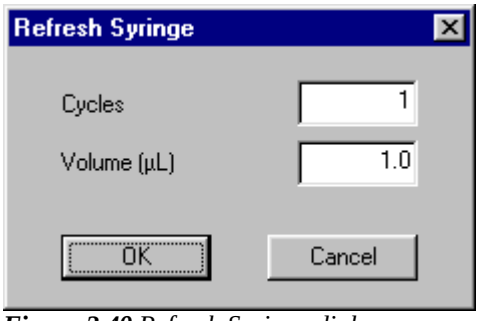


Figure 2.40 *Refresh Syringe dialog*

Refresh Syringe Refills the syringe with fresh, degassed, purge solvent.

Enter the number of **Cycles** and the replacement **Volume** and press **OK**. Waters recommend 12 Cycles and a volume of 600 µl.

Waters 2790 Plate Generator

To display the Plate Generator dialog, select **Plate Generator** from the **Waters2790** menu.

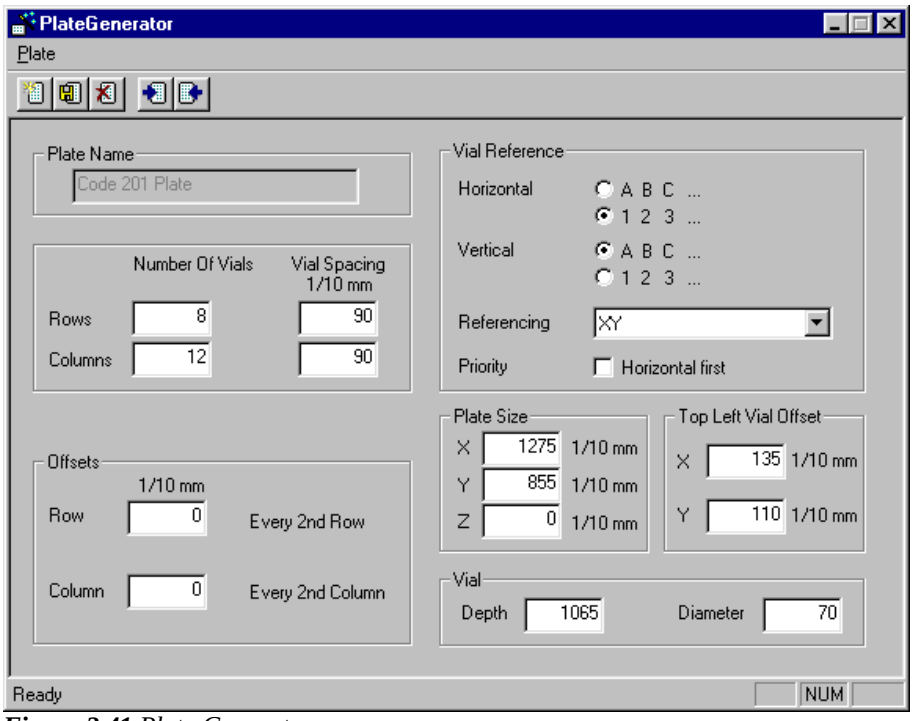


Figure 2.41 *Plate Generator*

Plate Name The name of the plate that is currently being edited.

Rows The number of vials in a row and the distance between each center.

Columns The number of vials in a column and the distance between each center.

Offsets Allows alternate vial rows or columns to be offset. **Note:** Entering a positive value will shift even numbered rows to the right and negative values will shift even numbered rows to the left.

Vial Reference Allows the user to select the way that the vial rows and columns are referenced, e.g. whether the rows are alphabetical or numerical.

Horizontal Sets the horizontal axis of the plate as either alphabetic (ABC) or numeric (123), when using XY referencing.

Vertical Sets the vertical axis of the plate as either alphabetic (ABC) or numeric (123), when using XY referencing.

Referencing This has three options

- XY which references the vials A1, B1 etc.
- Sequential Discontinuous which numbers the vials 1, 2, 3 across a row, left to right, and then starts the next row from the left again.
- Sequential Continuous which numbers the vials 1, 2, 3 across a row, left to right, then continues number the next row, right to left etc.

If the Waters 2790 autosampler is used with OpenLynx then the vial referencing must be set to either sequential continuous or sequential discontinuous.

Priority Check the **Horizontal First** box if samples are to be acquired horizontally across the plate.

If Referencing = X,Y, Horizontal = Letter, Vertical = Number and Horizontal Priority is checked, this will result in samples being acquired in the order A1, A2, A3. If the Horizontal Priority box is not checked samples will be acquired in the order 1A, 1B, 1C etc.

If Referencing = sequential continuous or discontinuous and Horizontal Priority is checked, this will result in samples being acquired from row 1 then row 2. If the Horizontal Priority box is not checked samples will be acquired from column 1 then column 2 etc.

Plate Size The size of the plate to its outside edges.

Top Left Vial Offset The measurement to the center of the first vial from the top left corner of the plate.

Vial The depth and diameter values are used for display only. They appear in the description for a single shot login on the OpenLynx Login screen.

Creating and Deleting Waters 2790 Plates

To create a new plate, press the  button. A new default plate is displayed, change the **Plate Name**, enter the appropriate values and press the save  button or select **Save Plate** from the **Plate** menu. New plates are saved to the MassLynx **Plates** directory.

To copy a plate, page through the list of saved plates using the  and  toolbar buttons. The **Previous Plate** and **Next Plate** options on the **Plate** menu perform the same operation. When the required plate is displayed change the **Plate Name**, enter the appropriate values and press the save  button or select **Save Plate** from the **Plate** menu. New plates are saved to the MassLynx **Plates** directory.

To delete a plate select the plate, by typing the name in the **Plate Name** box or by paging through as above, and press the delete  button or choose **Delete Plate** from the **Plate** menu.

Note: All of the spacings and the **vial section** are stored in 0.1 mm units.

Note: When defining a custom plate for use with a multi-injector the plate is required to be compatible with the position of the 8 needles of the autosampler.

- The Plate must have eight columns.
- The position of the vials should allow all eight needles to enter a separate vial.
- There should be no odd or even offsets for any of the vial positions.

Note: If the Plate currently selected on the Sample Configuration page is changed here, then **Reset Injector** should be selected from the **LC** menu to reset communications.

Note: All of the spacings and the **vial section** are stored in 0.1 mm units.

Vial Referencing Examples

The following tables show four examples of vial referencing for a simplified 4 × 3 vial plate.

	1	**2**	**3**	**4**	
A	1,A	2,A	3,A	4,A	**Horizontal: 123** **Vertical: ABC** **Referencing: XY** **Priority: Horizontal First Checked**
B	1,B	2,B	3,B	4,B	
C	1,C	2,C	3,C	4,C	

	1	**2**	**3**	**4**	
A	A,1	A,2	A,3	A,4	**Horizontal: 123** **Vertical: ABC** **Referencing: XY** **Priority: Horizontal First NOT Checked**
B	B,1	B,2	B,3	B,4	
C	C,1	C,2	C,3	C,4	

	1	**2**	**3**	**4**	
A	1	2	3	4	**Horizontal: N/A** **Vertical: N/A** **Referencing: Sequential Discontinuous** **Priority: Horizontal First Checked**
B	5	6	7	8	
C	9	10	11	12	

	1	**2**	**3**	**4**	
A	1	6	7	12	**Horizontal: N/A** **Vertical: N/A** **Referencing: Sequential Continuous** **Priority: Horizontal First NOT Checked**
B	2	5	8	11	
C	3	4	9	10	

Waters 2790 Bed Layout

Use the Bed Layout Editor to define the type, number, and location of the well plates on the 2790 plate carrier. To access the Bed Layout Editor, select **Bed Layout** from the **Waters2790** menu.

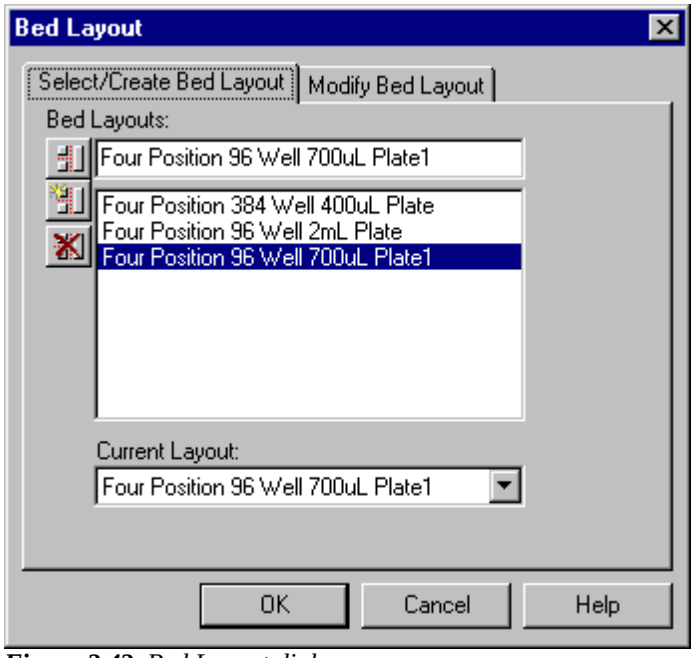


Figure 2.42 *Bed Layout dialog*

Bed Layouts Lists the available Bed Layouts.

Current Layout Specifies the bed layout currently in use.

- **To Delete A Bed Layout (Waters 2790)**

Highlight the bed layout to delete and press the  button. A dialog box will ask you to confirm the deletion. Press the **OK** button to delete the bed layout.

Note: You cannot delete the bed layout which is selected as the **Current Layout**.

- **To Create A New Bed Layout (Waters 2790)**

1. Highlight a bed layout similar to the one you want to create and press the  button to create a new layout. The layout appears in the **Bed Layouts** list as the same name with a 1 at the end, for example Six Position Microtiter1.

2. To change the name of the layout, type the new name into the Bed Layouts text box and press the  button. The name is updated in the Bed Layouts list box.

3. If the plate position or type needs changing select the **Modify Bed Layout** tab.

Note: New bed layouts are saved to the MassLynx **Racks** directory.

To Modify a Bed Layout (Waters 2790)

Use the Modify Bed Layout page to modify an existing bed layout. To access the Modify Bed Layout page, click the **Modify Bed Layout** tab. The Modify Bed Layout page shows a graphical representation of the selected bed layout. There are four plate positions in the 2790.

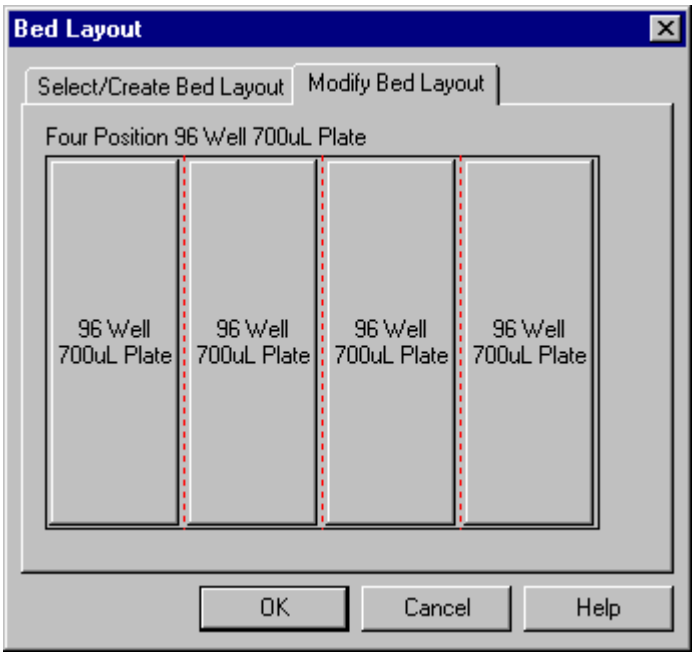


Figure 2.43 *Modify Bed Layout dialog*

Click the plate that you want to change to display the **Plate Position and Type** dialog.

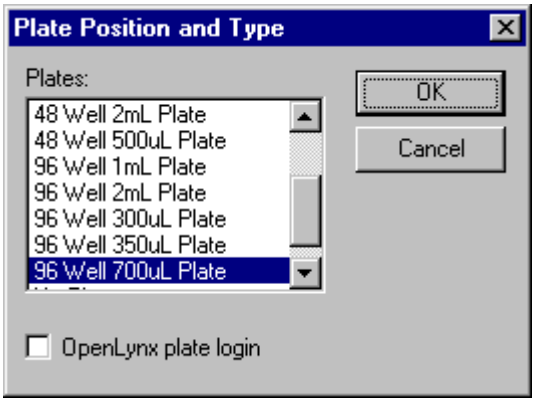


Figure 2.44 *Plate Position and Type dialog*

This dialog allows you to select a new plate from a list of possible options, and change its actual position on the bed. Select the plate type you want to use in the bed layout, then click **OK**.

OpenLynx plate login If this box is checked and **Use current MassLynx autosampler bed layout** is checked in the OpenLynx Manager program, then the plate at this position can only be used for plate login on the OpenLynx Login program.

Waters CapLC System Status Pages

The System Status pages display information about the state of the machine being controlled. These pages can be accessed within the Inlet Editor by selecting **Status** from the **View** menu or by pressing the  toolbar button.

- **Waters CapLC Solvent Status Page**

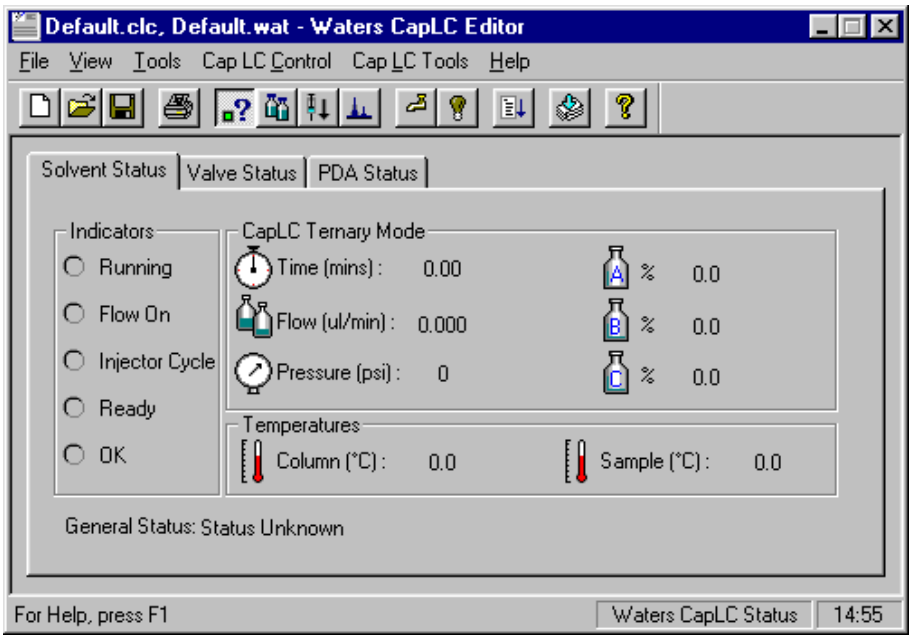


Figure 2.45 *Solvent Status page*

Indicators The Running, Pump On and Injector Cycle indicators at the left of the screen give information on the current status of the LC system. The OK and Ready Indicators become illuminated in red if the LC System has an error. Click on the red indicators to display more information on the cause of the malfunction.

Time This displays how long the method has been running.

Flow This displays the current flow rate as returned by the instrument.

Pressure This displays the current pressure in the instrument.

To the right of the Time, Flow and Pressure fields is a display of the solvent percentages at which the LC System is currently operating.

Column This displays the current temperature of the column.

Sample Temp This displays the current temperature of the sample.

Waters CapLC Valve Status Page

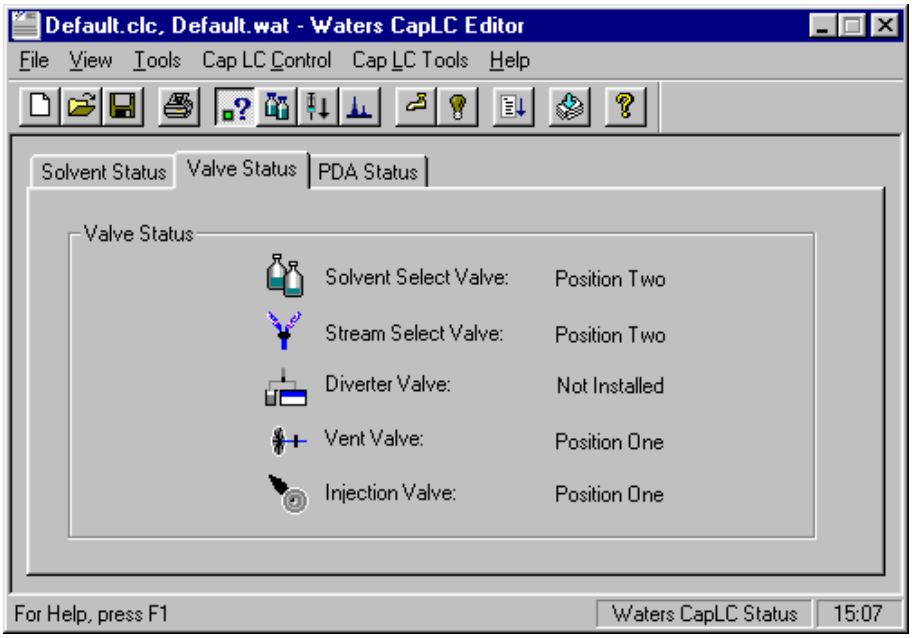


Figure 2.46 *Valve Status page*

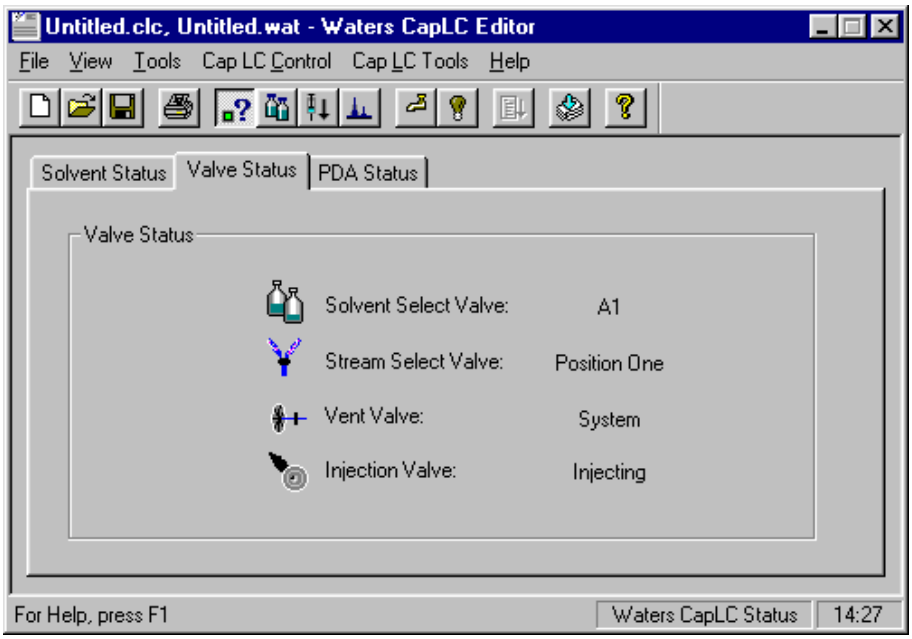


Figure 2.47 *Valve Status page*

This page shows what position the Valves are currently set to, if installed.

See the Waters Cap LC Users' Guide for details of the valves.

- **Waters CapLC PDA Status Page**

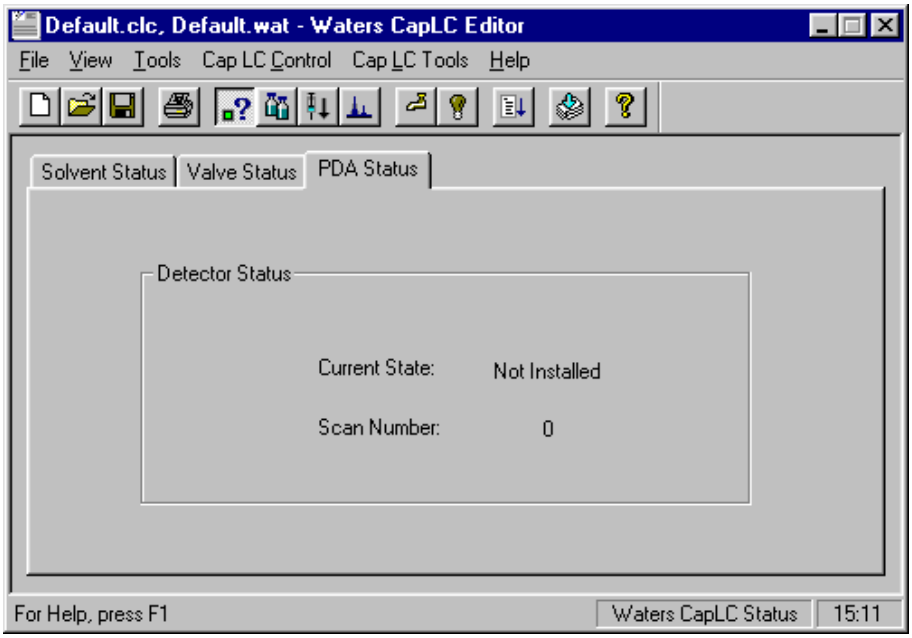


Figure 2.48 *PDA Status page*

Current State This displays the current state of the PDA Detector.

Scan Number When acquiring diode array data this displays the number of scans currently acquired.

Waters CapLC Pump

The Waters Pump pages can be accessed by selecting **WatersCapLC Pump** from the **View** menu on the Inlet Editor or by pressing the  toolbar button.

■ Waters CapLC Initial Conditions Page

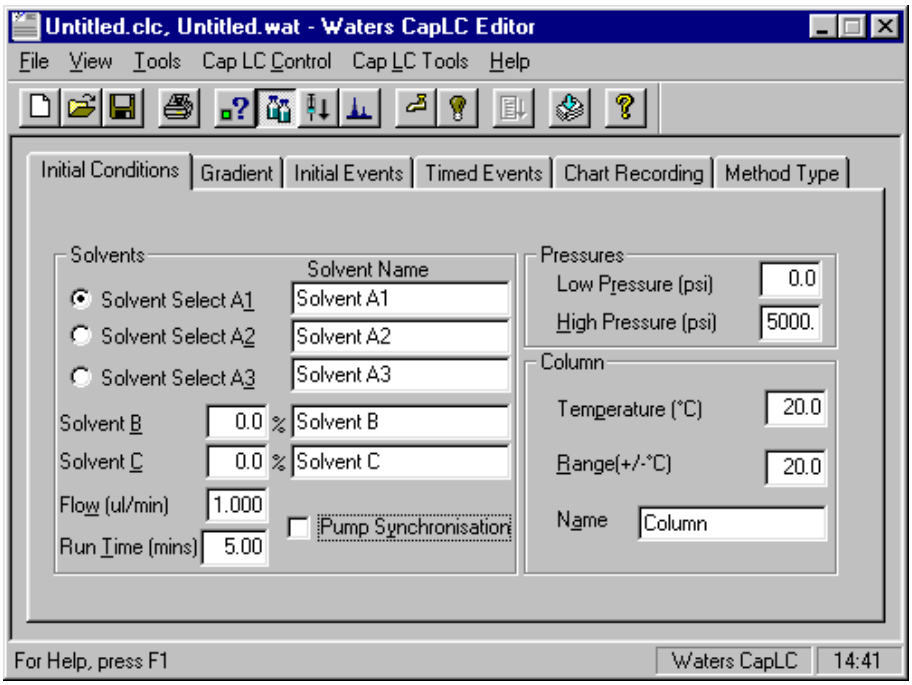


Figure 2.49 *Initial Conditions page*

Solvent Select A1 to A3 Select the solvent to deliver through Pump A.

Solvent B and C Enter the percentage of solvent flow from pump B and/or C (if installed).

Solvent Name Enter the name of the solvent in the corresponding solvent reservoir.

Flow Enter the total flow rate for the system in µl/min.

Run Time Enter the length of time (in minutes) until the next injection occurs.

Note: Run time is for the pump and autosampler only. Detectors have independent run times. The MS method run time must be greater than all other run time (see The Function List Editor chapter for details).

Note: If you are running a gradient or setting timed events, make sure you set the initial conditions Run Time to a value greater than or equal to the greatest Time value in the Gradient or Timed Events Table.

Low Pressure Enter the low-pressure limit for the system. If the system pressure falls below this limit, the flow stops and the LC Status error light turns red. Range: 0 to 4500 psi.

High Pressure Enter the high-pressure limit for the system. If the system pressure exceeds this limit, the flow stops and the LC Status error light turns red. Range: 0 to 5000 psi.

Temperature Enter the target operating temperature for the optional column heater. This value must be at least 5 °C above ambient. Range: 20 to 60 °C. Minimum setting: 5 °C above ambient.

Range Enter the maximum allowable temperature deviation from the value set for the column heater temperature. If the column heater temperature deviates beyond the specified range, the run stops and the LC Status error light turns red. Range: ±0.0 to ±10.0 °C.

Name Enter the name of the installed column.

■ Waters CapLC Gradient Page

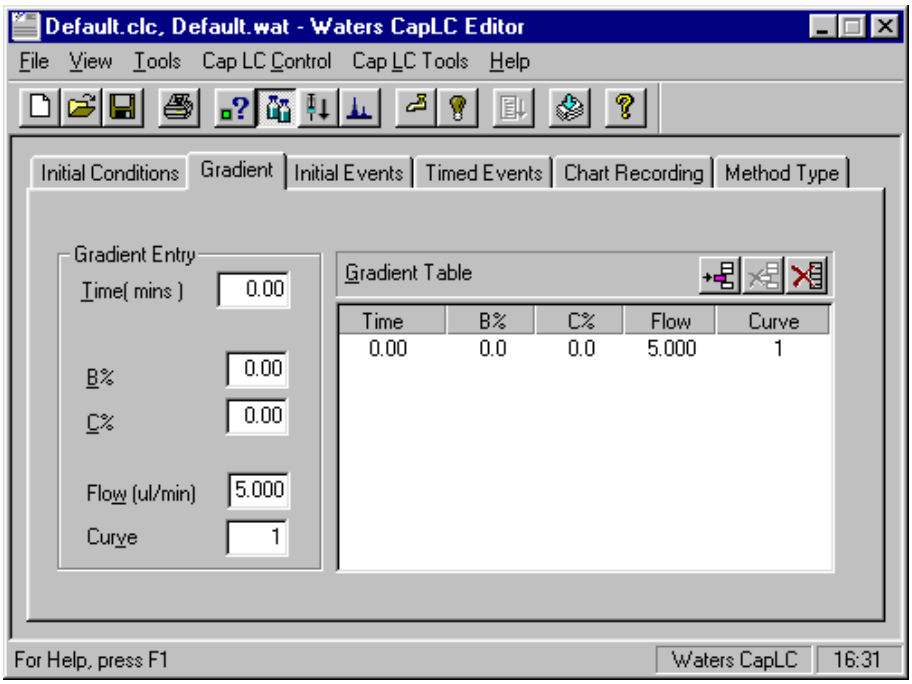


Figure 2.50 *Gradient page*

Use the Gradient Table to define conditions for a gradient run. For each row in the Gradient Table, define the percent composition of up to four solvents that are to be delivered at the desired flow rate for the specified time. Enter the number of the gradient curve required. This defines how changes to solvent percentages and flow rates take place over the elapsed time of each gradient segment (the time that elapses between the start time of one row and the start time of the next row).

Note: For an isocratic run, set the solvent percentages, run time and flow on the Initial Conditions page. Do **not** add any rows to the Gradient Table.

Waters CapLC Gradient Table Parameters

Time (mins) Specifies when the conditions (%A-%D, Flow, and Curve) for the row take effect. Make sure the Time for the first row is set to 0.00 to establish initial conditions for the gradient run. Range for rows other than row 1: 0.01 to 999.99 minutes.

B% and C% Specifies the percentage of solvent flow from each reservoir. For each row, the total of all solvents must equal 100%. Range: 0 to 100%.

Note: Percent flow for reservoir A is not displayed. Percent A is calculated as: 100% - (B% + C%)

Flow (µl/min) Specifies the total flow rate for the system.

Curve Specifies the rate of change of solvent composition and flow rate over time, based on the curve number and the length of the gradient segment. For more information, see Gradient Curves, below.

Waters CapLC Gradient Table Operation

To add a gradient, enter a time, percentage, flow rate and curve number in the relevant boxes and press the  toolbar button. **Note:** The first entry must have a time of 0.

To delete a single gradient click with left mouse button on a time in the list and press the  toolbar button.

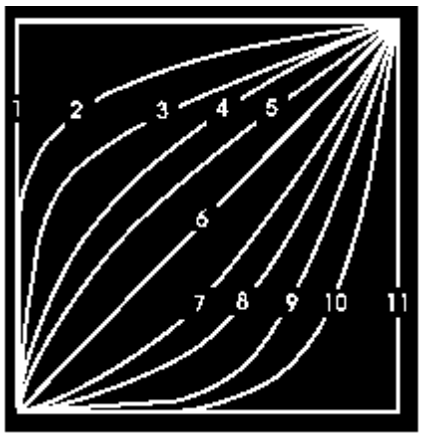
To delete all entries press the  toolbar button. This button is only available when there are entries in the timetable.

To modify a gradient select the required entry in the timetable. The values will then be displayed in the edit boxes above the timetable, and can be altered as appropriate. Once changed press  to re-enter the values into the timetable. If, however, you modify the time value such that it does not correspond to any existing entry in the timetable pressing  will result in a new entry being created in the timetable.

Gradient Curves

Curve Number	Effect
1	Immediately goes to specified conditions
2 to 5	Convex
6	Linear
7 to 10	Concave
11	Maintains start condition until next step

Curve Profiles



Waters CapLC Initial Events Page

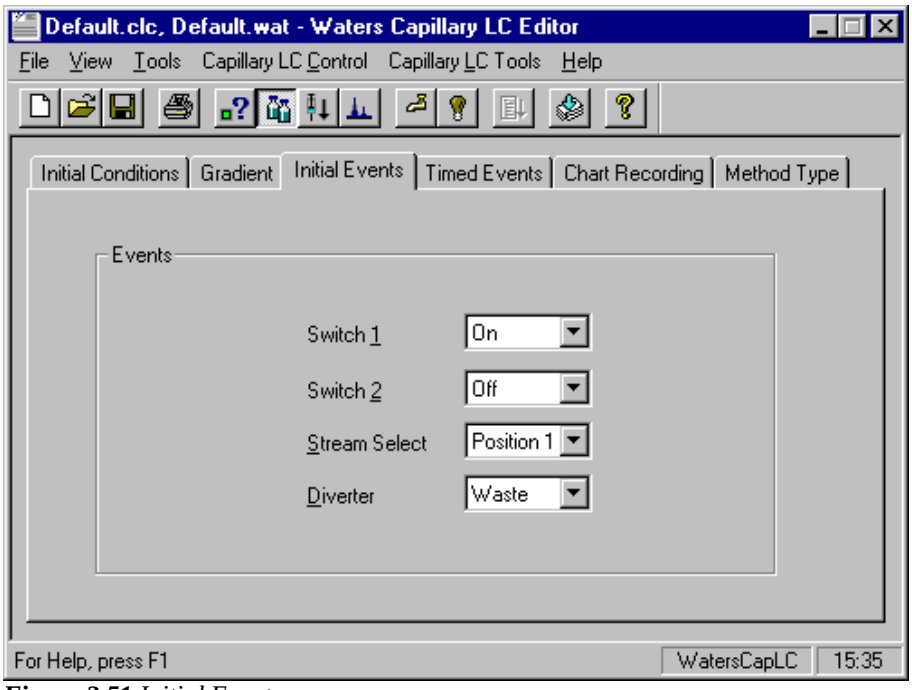


Figure 2.51 *Initial Events page*

Use the Initial Events page to set the initial condition of the two contact-closure output switches, the initial position of the stream select valve, and the initial position of the optional diverter valve.

Note: To change the settings of these switches and valves during a run, use the Timed Events Table.

Switch 1 and **2** Select the initial state of contact-closure Switch 1 and 2 from the drop down list boxes.

Stream Select Select the initial state of the stream select valve (Position 1 or 2) from the drop down list box.

Diverter Select the initial position of the optional diverter valve (System or Vent) from the drop down list box.

■ Waters CapLC Timed Events Page

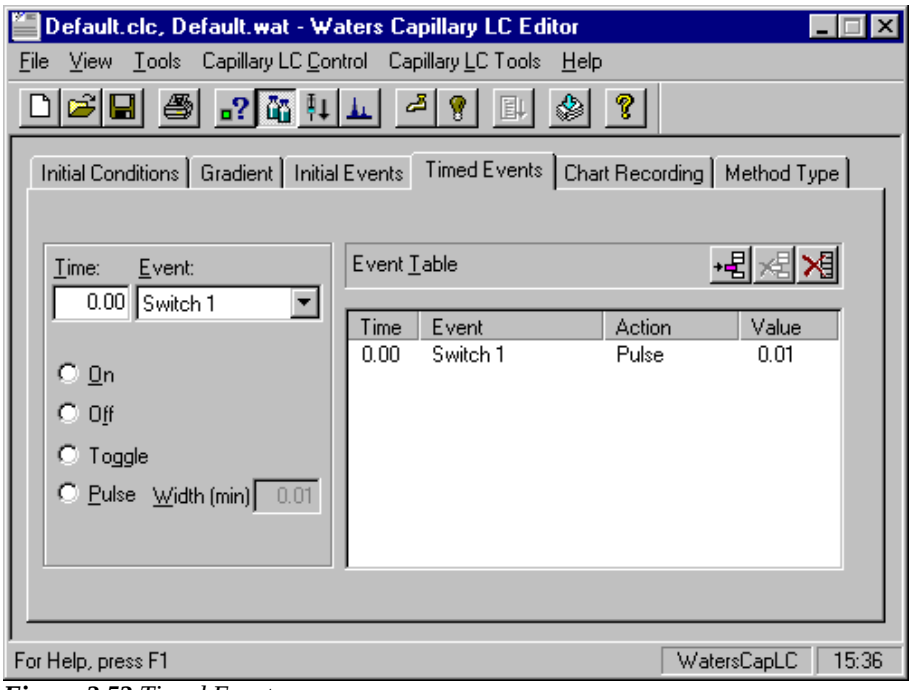


Figure 2.52 *Timed Events page*

Use the Event Table to program up to 16 events (both external and internal). The external events are triggered by four contact closures (relays) through output terminals (S1–S4) on the 2790 Separations Module. The internal events are used to control the sample compartment temperature, column heater temperature, and to prime and flush the 2790 Separations Module. Events can be triggered more than once and multiple events can be triggered simultaneously.

Waters CapLC Event Table Parameters

Time Enter the time (after injection) at which the event starts. Event rows are sorted automatically by time. **Note:** Different events can be programmed to occur at the same time. Range: 0.00 to 999.99 min.

Event Select the type of event signal: one of the two contact-closure output switches (Switch1or Switch 2), or one of the internal events (Set temperature, Stream Select or Vent Valve). Choose from these event types to program up to 16 events. **Note:** The same event can be programmed more than once. Available choices:

- **Switch 1** and **2** Corresponds to terminal strip positions S1 and S2 on the rear of the unit. Activating a Switch event triggers a contact closure for controlling an external device. Select a switch event and a state for the switch (On, Off, Toggle, Pulse or No Change). This state appears in the Action column of the table (see Switch States, below). **Note:** If Pulse is selected for a switch state the duration of the pulse must be entered in the **Width** (min) field.

- **Set Temperature** Specifies the temperature of an optional column heater. If Set Temperature is selected for a switch state the temperature in (°C) must be entered in the **Column Temperature** field. **Note:** When this event occurs, the temperature of the column heater changes from the value set on the Initial Conditions page to the value set for the event. When the event times out, the temperature returns to the value on the Initial Conditions page value.

- **Stream Select** (1 or 2) Specifies the position of the stream select valve.

- **Vent Valve** (System or Vent) Specifies the position of the vent valve.

Waters CapLC Switch States

- **On** – Turns on a contact closure that triggers an external or internal event. With this function, the contact closure remains closed until an Off function is sent.
- **Off** – Turns off the contact closure for the event. With this function, the contact closure is broken.
- **Toggle** – Changes the current state of the switch.
- **Pulse** – Transmits a single On/Off pulse. The contact closure is maintained for the time entered in the **Width** box. Range: 0.01 to 100.00 minutes.
- **No Change** – Leaves the switch in its current state.

Waters CapLC Event Table Operation

To add an event, enter a time, event, action and value in the relevant boxes and press the  toolbar button. Note the first entry must have a time of 0.

To delete a single event click with left mouse button on a time in the list and press the  toolbar button.

To delete all entries press the  toolbar button. This button is only available when there are entries in the timetable.

To modify an event select the required entry in the timetable. The values will then be displayed in the edit boxes, and can be altered as appropriate. Once changed press  to re-enter the values into the timetable. If, however, you modify the time value such that it does not correspond to any existing entry in the timetable pressing  will result in a new entry being created in the timetable.

Waters CapLC Chart Recording Page

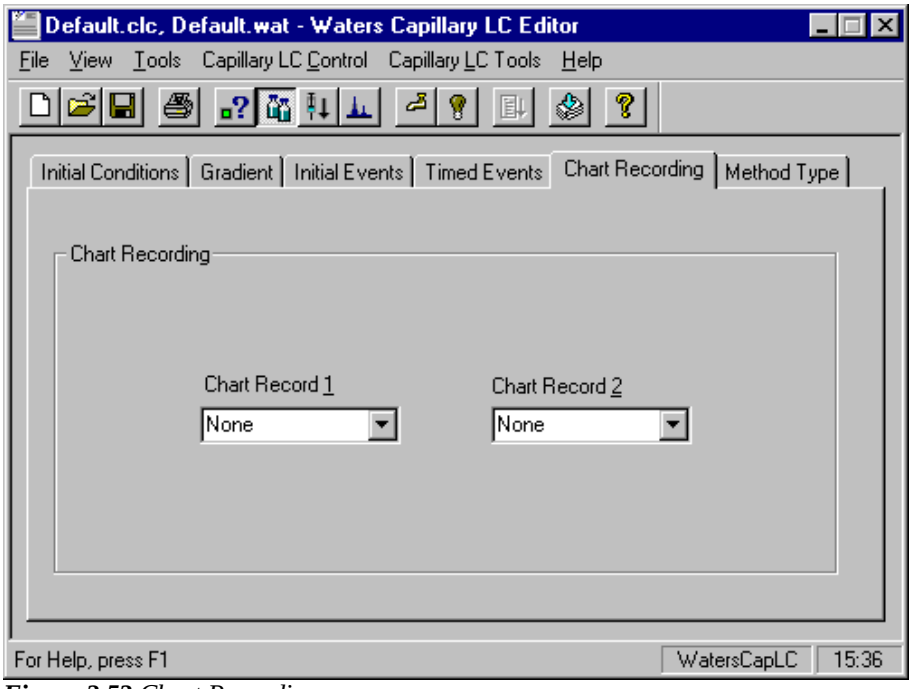


Figure 2.53 *Chart Recording page*

Use the Chart Recording page to select up to two analog signals to be output to an external device such as an integrator or strip-chart recorder. Select one of the following the signals to output, from the drop down list box.

- None
- Flow
- Pressure
- Percent A, B, or C
- Column temperature

Note: To record a signal, you need to connect each external device to the appropriate Chart Out terminal pair on the rear of the unit. Refer to the Waters CapLC System Installation and Maintenance Guide for installation and specification details.

Waters CapLC Method Type Page

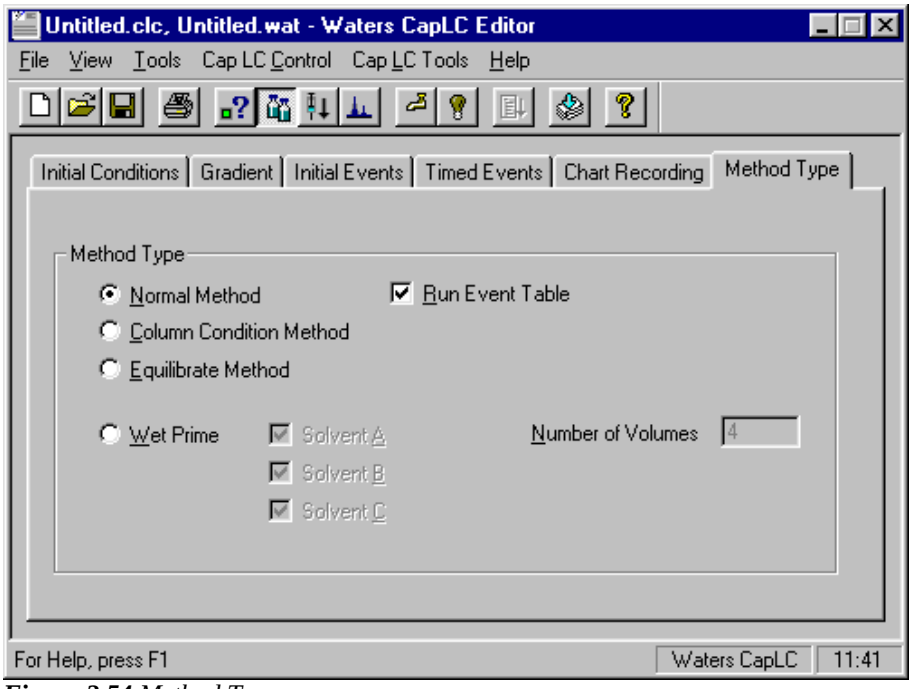


Figure 2.54 *Method Type page*

Method Type Specifies the type of method to create. Select one of:

- **Normal Method** The Method Type used for standard injections. Ensure that the Method Type is set to **Normal** unless you are performing one of the procedures listed below.
- **Column Condition Method** Runs solvent through the column without injecting samples or running the Events table. Solvent is delivered using the gradient table specified in the Gradient page.
- **Equilibrate Method** Delivers solvents and maintains solvent parameters using the values defined on the Initial Conditions page.
- **Wet Prime** Replaces solvent in the tubing with fresh solvent from the reservoirs through the Prime port of the inject valve to waste. Use a Wet Prime Method when changing the solvents in the system. Check the boxes for the solvent lines to prime, and the number of loop volumes to use.

  Waters recommends starting the wet prime using the solvent with the lowest viscosity to help purge air from the lines, especially if the in-line vacuum degasser is installed.

  Note: If the solvent lines in the CapLC are dry, you must perform the dry prime procedure before performing a wet prime.

Waters CapLC Autosampler

These pages are used to set parameters specific to the Autosampler, to access them select **WatersCapLC AutoSampler** from the **View** menu or press the  toolbar button.

■ Waters CapLC AutoSampler Page

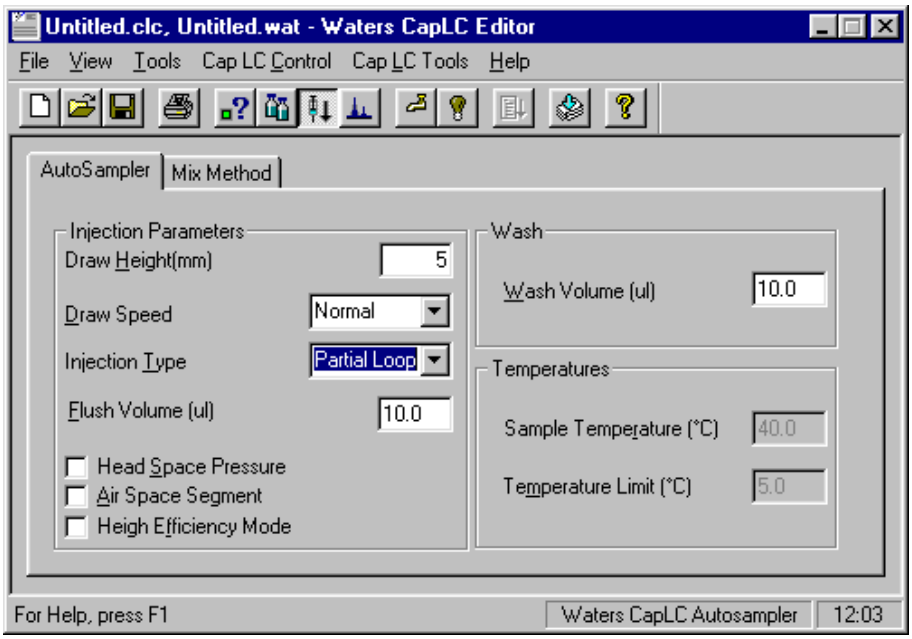


Figure 2.55 *CapLC AutoSampler page*

Draw Height Adjusts the depth of the needle tip to accommodate for sedimented samples. A value of 0 corresponds to the top of the plate carrier. Range: 0 to 40 mm.

Draw Speed Select the draw rate of the syringe from the drop down list box. The different rates accommodate for samples of varying viscosity. The rate for each selection is dependent on the size of the installed syringe. The table below shows the draw rates for each selection.

	Draw Rate for 25 µl Syringe	**Draw Rate for 100 µl Syringe**	**Draw Rate for 250 µl Syringe**	**Draw Rate for 500 µl Syringe**
Fast	94 µl/min	375 µl/min	940 µl/min	1875 µl/min
Normal	63 µl/min	250 µl/min	625 µl/min	1250 µl/min
Slow	32 µl/min	375 µl/min	315 µl/min	625 µl/min

Injection Type Select one of the following injection types from the drop down list box:

- **Full Loop** – The sample loop is completely filled.
- **Partial Loop** – The sample loop is partially filled with the volume defined in the Sample List. The value in the Sample List must not exceed the Full Loop volume.
- **µl Pickup** – The sample loop is filled with only the amount of sample to be injected (resulting in no sample loss). Sample is transported into the loop by transport liquid (mobile phase) from the transport vial.
- **Manual** – Specifies that the manual injector is used (the autosampler is disabled). Switching the manual injector to the Inject position initiates any programmed gradients and/or timed events.

Flush Volume Enter the volume (in microliters) of sample taken from a vial before the loop is filled with sample. This flushes out previous samples.

Head Space Pressure If this box is checked the prepuncturing needle will put approximately 0.5 bar of pressure on the sample to stop formation of air or vapour bubbles. Enable this parameter only when using sample vials with air-tight caps.

Air Space Segment If this box is checked an air segment is added to the front of the flush volume to minimize dilution and bandspreading and reduce the amount of flush volume required. In Full and Partial Loop modes, the air segment is flushed to waste; in µl Pickup mode, the air segment is injected. Disable this parameter if the air segment causes problems in µl Pickup mode.

High Efficiency Mode If this box is checked the sample loop will be taken out of the flow stream after the sample has been flushed, but before the gradient front reaches the injection valve.

Wash Volume Enter the volume (in microliters) of wash solvent used to clean the needle and buffer tubing.

Sample Temperature Enter the target operating temperature for the optional sample heater/cooler. Range: 4.0 to 40.0 °C.

Temperature Limit Enter the maximum allowable temperature deviation from the value set for the Sample Temperature. If the sample temperature deviates beyond the specified range, the LC Status error light turns red and the run stops.
Range: ±1.0 to ±20.0 °C.

- **Waters CapLC Mix Method Page**

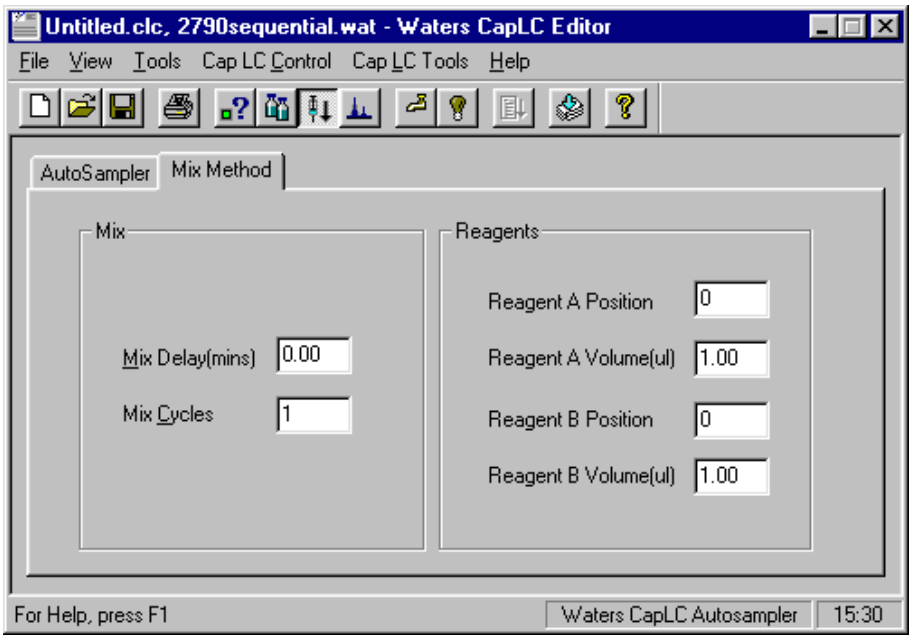


Figure 2.56 *Mix Method page*

Mix Delay Enter the delay time before mixing, in minutes. A value of 0 corresponds to the top of the plate carrier. Range: 0 to 99.9 mins.

Mix Cycles Enter the number of times to perform the Mix operation.

Reagent Position 1 Enter the position of the first reagent to mix.

Volume Reagent 1 Enter the volume of reagent 1 to mix.

Reagent Position 2 Enter the position of the second reagent to mix.

Volume Reagent 2 Enter the volume of reagent 2 to mix.

Waters CapLC Bed Layout

Use the Bed Layout Editor to define the type, number, and location of the well plates on the CapLC plate loader. To access the Bed Layout Editor, select **Bed Layout** from the **Cap LC Tools** menu.

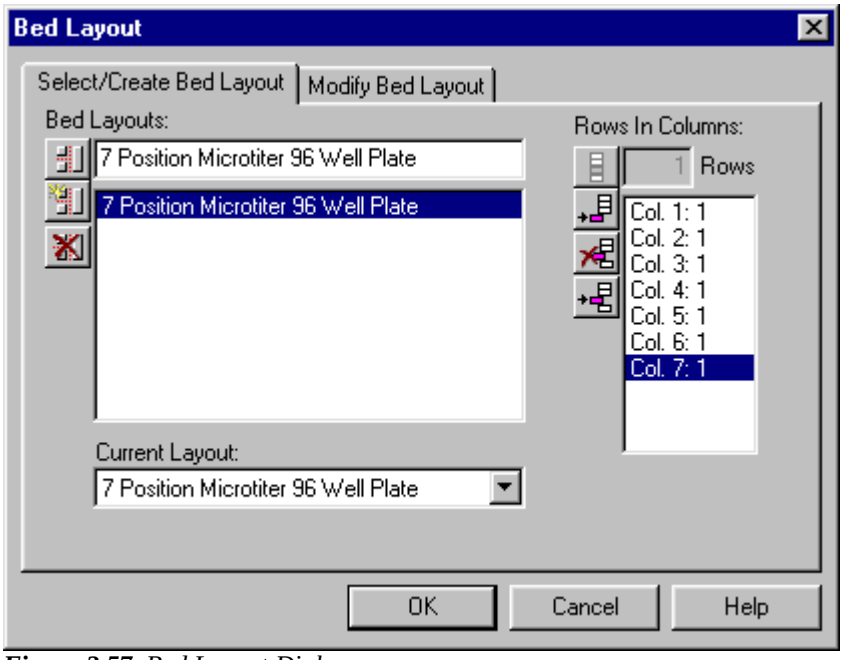


Figure 2.57 *Bed Layout Dialog*

Bed Layouts Lists the available Bed Layouts.

Current Layout Specifies the bed layout currently in use.

- **To Delete A Bed Layout (Waters CapLC)**

Highlight the bed layout to delete and press the  button. A dialog box will ask you to confirm the deletion. Press the **OK** button to delete the bed layout.

Note: You cannot delete the bed layout which is selected as the **Current Layout**.

- **To Create A New Bed Layout (Waters CapLC)**

1. Highlight a bed layout similar to the one you want to create and press the  button. The layout appears in the **Bed Layouts** list as the same name with a 1 at the end, for example Six Position Microtiter1.

2. To change the name of the layout, type the new name into the Bed Layouts text box and press the  button. The name is updated in the Bed Layouts list box.

3. If the plate position or type needs changing select the **Modify Bed Layout** tab.

Note: New bed layouts are saved to the MassLynx **Racks** directory.

To Modify a Bed Layout (Waters CapLC)

Use the Modify Bed Layout page to modify an existing bed layout. To access the Modify Bed Layout page, click the **Modify Bed Layout** tab. The Modify Bed Layout page shows a graphical representation of the selected bed layout.

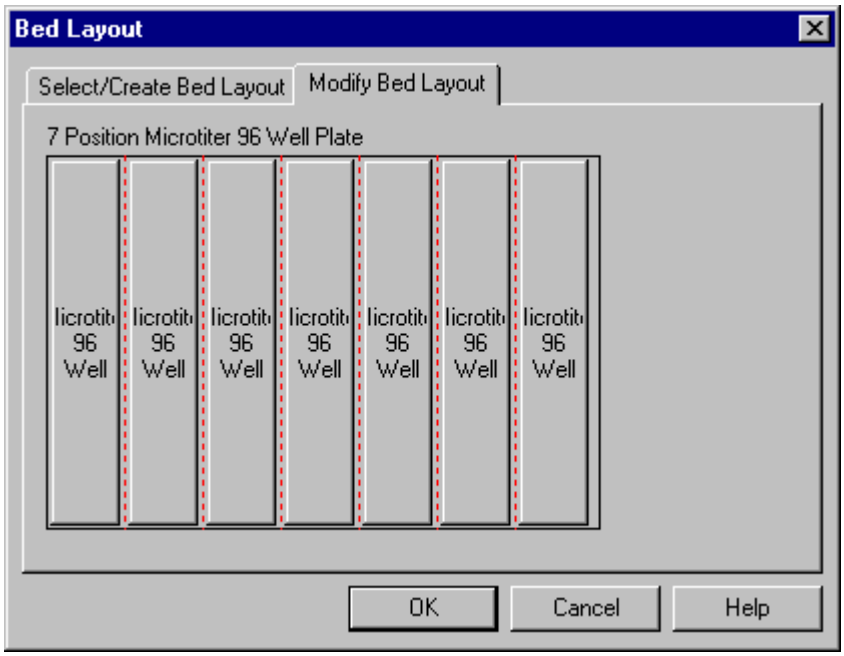


Figure 2.58 *Modify Bed Layout Dialog*

Click on the plate that you want to change to display the **Plate Position and Type** dialog.

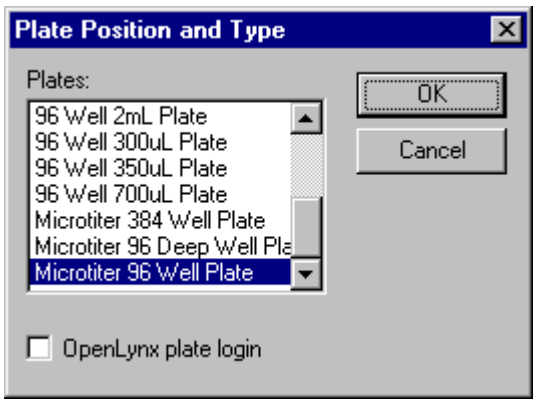


Figure 2.59 *Plate Position and Type Dialog*

This dialog allows you to select a new plate from a list of possible options, and change its actual position on the bed. Select the plate type to use in the bed layout, then click **OK**.

OpenLynx plate login If this box is checked and **Use current MassLynx autosampler bed layout** is checked in the OpenLynx Manager program, then the plate at this position can only be used for plate login on the OpenLynx Login program.

- **Other Bed Layout Options (Waters CapLC)**

1. To append a new column, press the  button.
2. To delete the current column press the  button.
3. To insert a column, click on the column before which you want to insert and press the  button. **Note:** The column inserted will have the same number of rows as the column highlighted.
4. **Note:** The number of rows in a column cannot be changed and so the  button is greyed out.

Waters CapLC Plate Generator

To display the Plate Generator dialog, select **Plate Generator** from the **Cap LC Tools** menu.

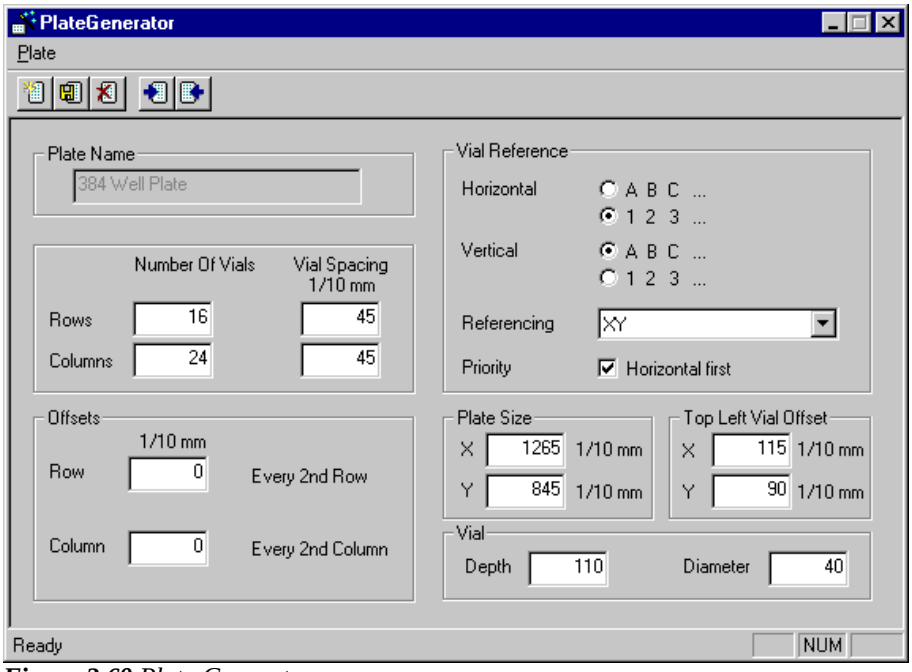


Figure 2.60 *Plate Generator*

Plate Name The name of the plate that is currently being edited.

Rows The number of vials in a row and the distance between each center.

Columns The number of vials in a column and the distance between each center.

Offsets Allows alternate vial rows or columns to be offset. **Note:** Entering a positive value will shift even numbered rows to the right and negative values will shift even numbered rows to the left.

Vial Reference Allows the user to select the way that the vial rows and columns are referenced, e.g. whether the rows are alphabetical or numerical.

Horizontal Sets the horizontal axis of the plate as either alphabetic (ABC) or numeric (123), when using XY referencing. Default: numeric.

Vertical Sets the vertical axis of the plate as either alphabetic (ABC) or numeric (123), when using XY referencing. Default: alphabetic.

Referencing This has three options

- XY which references the vials A1, B1 etc.
- Sequential Discontinuous which numbers the vials 1, 2, 3 across a row, left to right, and then starts the next row from the left again.
- Sequential Continuous which numbers the vials 1, 2, 3 across a row, left to right, then continues number the next row, right to left etc.

If the Waters CapLC autosampler is used with OpenLynx then the vial referencing must be set to either sequential continuous or sequential discontinuous.

Priority Check the **Horizontal First** box if samples are to be acquired horizontally across the plate.

If Referencing = X,Y and Horizontal First is checked, then the horizontal value be read first when referencing a vial (1,A). If Horizontal First is not selected, then the vertical value be read first when referencing a vial (A,1). Default: Horizontal First selected.

If Referencing = Sequential Continuous or Discontinuous and Horizontal First is checked, then vials will be numbered horizontally. This will result in samples being acquired from row 1 then row 2. If Horizontal First is not checked, then vials will be numbered vertically. This will result in samples being acquired from column 1 then column 2 etc.

Default: Horizontal First selected.

Plate Size The size of the plate to its outside edges.

Top Left Vial Offset The measurement to the center of the first vial from the top left corner of the plate.

Vial The depth and diameter values are used for display only. They appear in the description for a single shot login on the OpenLynx Login screen.

Creating and Deleting Waters CapLC Plates

To create a new plate press the  button. A new default plate is displayed, change the **Plate Name**, enter the appropriate values and press the save  button or select **Save Plate** from the **Plate** menu. New plates are saved to the MassLynx **Plates** directory.

To copy a plate, page through the list of saved plates using the  and  toolbar buttons. The **Previous Plate** and **Next Plate** options on the **Plate** menu perform the same operation. When the required plate is displayed change the **Plate Name**, enter the appropriate values and press the save  button or select **Save Plate** from the **Plate** menu. New plates are saved to the MassLynx **Plates** directory.

To delete a plate select the plate, by typing the name in the **Plate Name** box or by paging through as above, and press the delete  button or choose **Delete Plate** from the **Plate** menu.

Note: All of the spacings and the **vial section** are stored in 0.1 mm units.

Note: When defining a custom plate for use with a multi-injector the plate is required to be compatible with the position of the 8 needles of the autosampler.

- The Plate must have eight columns.
- The position of the vials should allow all eight needles to enter a separate vial.
- There should be no odd or even offsets for any of the vial positions.

Note: If the Plate currently selected on the Sample Configuration page is changed here, then **Reset Injector** should be selected from the **LC** menu to reset communications.

Note: All of the spacings and the **vial section** are stored in 0.1 mm units.

Vial Referencing Examples

The following tables show four examples of vial referencing for a simplified 4 × 3 vial plate.

	1	**2**	**3**	**4**	
A	1,A	2,A	3,A	4,A	**Horizontal: 123** **Vertical: ABC** **Referencing: XY** **Priority: Horizontal First Checked**
B	1,B	2,B	3,B	4,B	
C	1,C	2,C	3,C	4,C	

	1	**2**	**3**	**4**	
A	A,1	A,2	A,3	A,4	**Horizontal: 123** **Vertical: ABC** **Referencing: XY** **Priority: Horizontal First NOT Checked**
B	B,1	B,2	B,3	B,4	
C	C,1	C,2	C,3	C,4	

	1	**2**	**3**	**4**	
A	1	2	3	4	**Horizontal: N/A** **Vertical: N/A** **Referencing: Sequential Discontinuous** **Priority: Horizontal First Checked**
B	5	6	7	8	
C	9	10	11	12	

	1	**2**	**3**	**4**	
A	1	6	7	12	**Horizontal: N/A** **Vertical: N/A** **Referencing: Sequential Continuous** **Priority: Horizontal First NOT Checked**
B	2	5	8	11	
C	3	4	9	10	

Waters CapLC Plate Loader

To display the Plate Loader dialog, select **Plate Loader** from the **Cap LC Tools** menu.

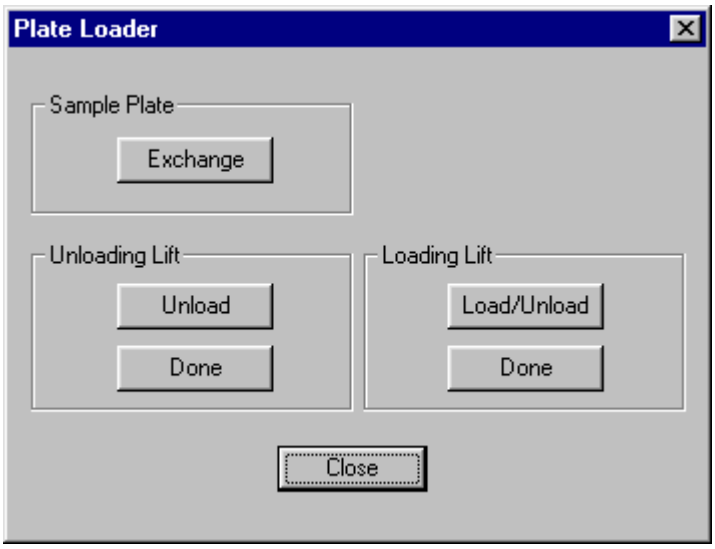


Figure 2.61 *Plate Loader*

The Plate Loader dialog is used when a plate needs to be changed.

Waters CapLC PDA Detector

This page is used to set parameters specific to the UV detector, to access it select **WatersCapLC PDA Detector** from the **View** menu or press the  toolbar button.

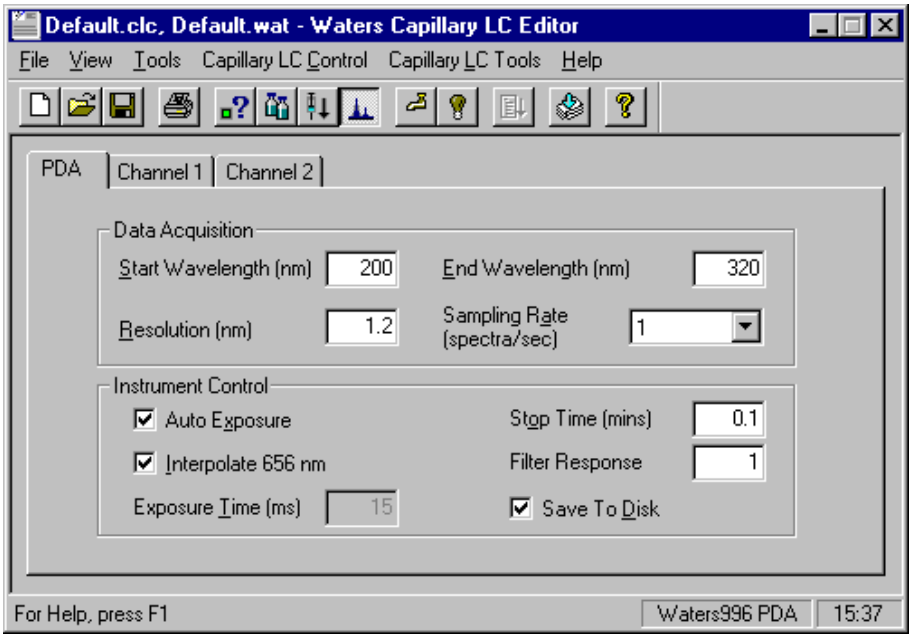


Figure 2.62 *CapLC PDA Detector Configuration page*

Start Wavelength Enter the wavelength at which to start acquiring data.

Range (with Resolution set to 1.2): 190.0 nm to 800.0 nm. Range (at all other Resolution settings): 190.0 + (Resolution/2) to 800.0 – (Resolution/2). Default: 200 nm.

End Wavelength Enter the wavelength at which to stop acquiring data.

Range with Resolution set to 1.2: Start Wavelength to 800.0 nm. Range at all other Resolution settings: Start Wavelength + Resolution to 800.0 nm – Resolution/2.

Resolution Enter the number of diodes to be averaged together as a single spectral data point. To differentiate closely related spectra and obtain greater spectral resolution, use a small resolution number. Be aware, however, that a small resolution value generates more data points and therefore requires more disk space than a large resolution value. Find a resolution value just small enough to identify spectral features. Range: 1.2 to 24.0 nm in multiples of 1.2.

Sampling Rate Select the acquisition rate in spectra per second from the drop down list box. For good integration and quantitation, acquire 15 to 20 spectra across a peak.

Auto Exposure Check this box to enable the detector optics to calculate the optimum exposure time needed to recharge the diodes based on the lamp energy, the lamp spectrum and the selected wavelength range.

Tip: Enable Auto Exposure for most routine analyses.

Interpolate Check this box to instruct the detector to ignore the signal from the photodiode at 656 nm and to interpolate a value from the adjacent diodes. This prevents over-saturation at 656 nm (Balmer line for deuterium).

If this box is not checked the detector reports the signal from the photodiode at 656 nm. Disable this parameter only if you are working with compounds that absorb in the 656 nm range.

Note: If this parameter is unchecked, the deuterium lamp high emission line at 656 nm may cause spectral artifacts and autoexposure errors.

Exposure Time Enter the length of time in milliseconds that the photodiodes are exposed to light before they are read. This parameter is not accessible if Auto Exposure is checked. Range: 11.00 to 500.00 ms.

Stop Time Enter the time, in minutes after injection, when the PDA will stop scanning. *This value is independent of the instrument method run time.*

Filter Response Enter the response time (in seconds) for filtering acquired data. The filter is an enhanced rolling average filter applied to absorbance data from the PDA detector before the data is sent to the MassLynx software. The filter reduces high-frequency noise across the entire wavelength range specified for the acquisition. High values decrease peak response. Range: 0 to 3.

Save to Disk Check this box to save the Photo Diode Array data to the raw datafile. If this data is not required for further processing then uncheck the box, the data is not saved to disk thus reducing the size of the file.

■ Waters CapLC Channel Detector Configuration Pages

The Channel 1 and Channel 2 pages contain the same information. Select the page relevant to the channel required, by clicking on the tab.

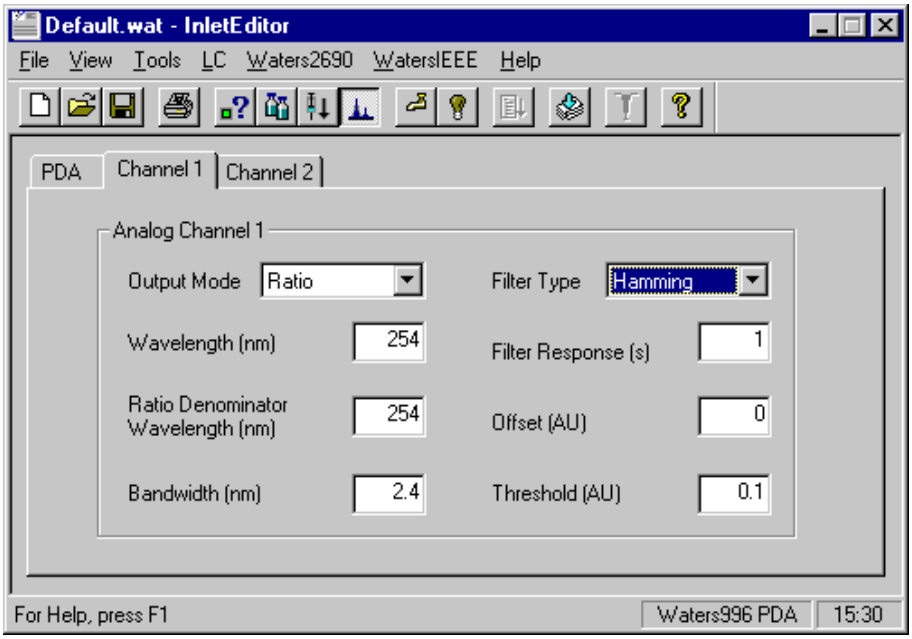


Figure 2.63 *Channel 1 Detector Configuration page*

Output Mode Select one of:

- **Off –** no analog output signal.
- **Absorbance –** Output represents absorbance at the wavelength specified by the Wavelength parameter (see below).

  Note: Ratio Denominator Wavelength and **Threshold** parameters are not accessible when Absorbance mode is selected.

- **Ratio** – Output represents the ratio of absorbances at two wavelengths. The numerator wavelength is specified by the Wavelength parameter, and the denominator wavelength is specified by the Ratio Denominator Wavelength parameter (see below).

Wavelength Enter the output wavelength. In Ratio mode, the absorbance at the Wavelength is used to calculate ratio in the formula:

> Ratio = Absorbance at Wavelength/Absorbance at Ratio Denominator Wavelength

Wavelength must be within the wavelength range specified by the Start Wavelength and End Wavelength parameters on the PDA page.

Range when Resolution is set to 1.2: Start Wavelength to End Wavelength. Range at all other Resolution settings: Start Wavelength + (Bandwidth/2) to End Wavelength – (Bandwidth/2).

Ratio Denominator Wavelength Enter the denominator wavelength (in nanometers) for the analog output channel. Ratio Denominator Wavelength must be within the wavelength range specified by the Start Wavelength and End Wavelength parameters in the 996 PDA page.

Bandwidth Enter the spectral bandwidth of the analog output channel. Range: 1.2 to 24.0 nm in multiples of 1.2.

Filter Type Select the filter type (Hamming or Single Pole) from the drop down list box for use on the analog output channel. The Hamming filter is designed to create the same degree of peak-height degradation as the Single Pole filter for the same response time, but enhances filtering of high-frequency noise.

Filter Response Enter the response time in seconds for the Filter Type specified above. Range: 0 to 5 seconds.

Offset If required enter an offset to the analog output channel. Range: –0.2 to 2.0 AU.

Threshold Enter a threshold above which the ratio (Wavelength / Ratio Denominator Wavelength) must be to be valid data. The range is –0.1 to 2.0 AU.

Note: If no ratio is plotted (one or both channels are below the current Threshold), enter a lower Threshold value.

Waters 515 and 1525 Pumps

The Waters 515 and 1525 Pump pages can be accessed by selecting **Waters 515 Pump** or **Waters 1525 Pump** from the **View** menu on the Inlet Editor or by pressing the  toolbar button.

- **Waters 515/1525 Initial Conditions Page**

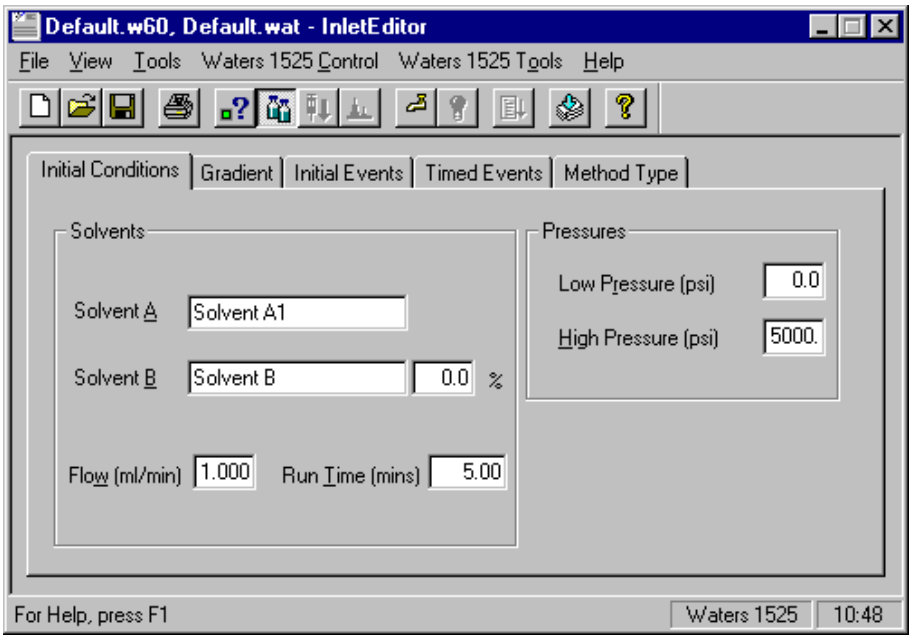


Figure 2.64 *Initial Conditions page*

Solvent A Enter the name of the solvent that will be delivered through Pump A.

Solvent B Enter the name of the solvent that will be delivered through Pump B and enter the percentage of the solvent flow from Pump B.

Flow (ml/min) Enter the total flow rate for the solvent delivery system. Range: 1 to 10 ml/min.

Run Time Enter the time in minutes that the method will run, from the point of injection.

Note: If you are running a gradient or setting timed events, make sure the **Run Time** value is greater than, or equal to the greatest **Time** value, specified on the Gradient or Timed Events pages.

Low Pressure Enter the low pressure limit for the system. If the pressure falls below this limit, the solvent flow will stop and the LC status light will turn red.

High Pressure Enter the high pressure limit for the system. If the pressure exceeds this limit, the solvent flow will stop and the LC status light will turn red.

Waters 515

If you selected a Waters 515 Pump, the **Auxiliary Pump Solvent** options are displayed:

Flow (ml/min) Enter the total flow rate for the auxiliary solvent delivery system. Range: 1 to 10 ml/min.

Name Enter the name of the solvent that will be delivered through the auxiliary pump.

- **Waters 515/1525 Gradient Page**

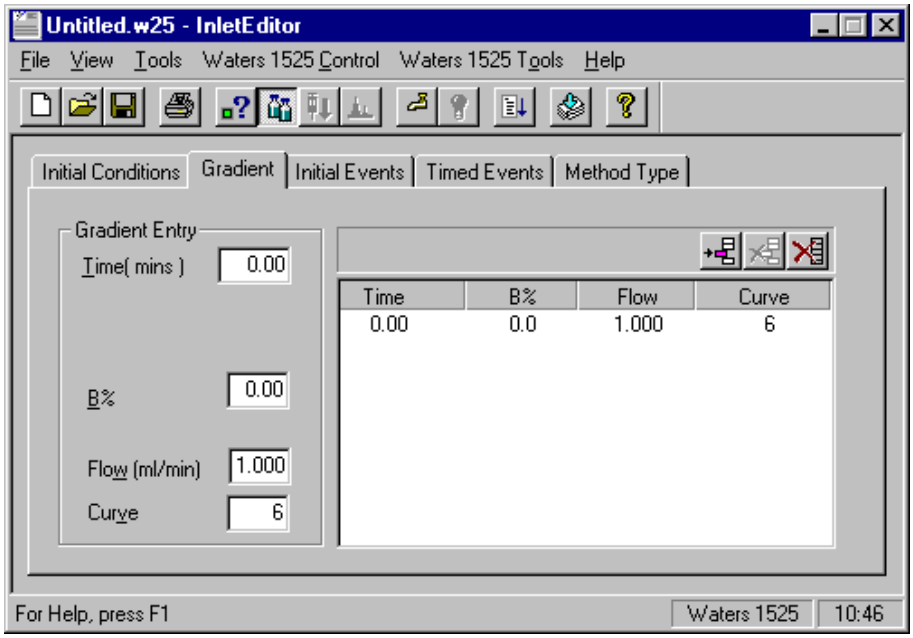


Figure 2.65 *Gradient page*

Use the Gradient Table to define conditions for a gradient run. For each row in the Gradient Table, you need to define the % composition of up to two solvents that are to be delivered at the desired flow rate for the specified **Time**.

Note: For an isocratic run, set the solvent percentages, run time and flow, on the Initial Conditions page. Do not add any rows to the Gradient Table.

To add a gradient, enter a time and percentage in the relevant boxes and press the  toolbar button. **Note:** The first entry must have a time of 0.

To delete a single gradient, click with left mouse button on a time in the list and press the  toolbar button.

To delete all entries press the  toolbar button. This button is only available when there are entries in the timetable.

To modify a gradient, select the required entry in the timetable. The values will then be displayed in the edit boxes to the left of the timetable, and can be altered as appropriate. Once changed press  to re-enter the values into the timetable. If, however, you modify the time value such that it does not correspond to any existing entry in the timetable pressing  will result in a new entry being created in the timetable.

Flow Enter the flow rate for the solvent delivery system.

Curve Enter the number of the gradient curve required. This sets the rate at which the solvent is to change to the new proportions and/or flow rates. See the Waters Operator's Guide for a list of values.

■ Waters 515/1525 Initial Events Page

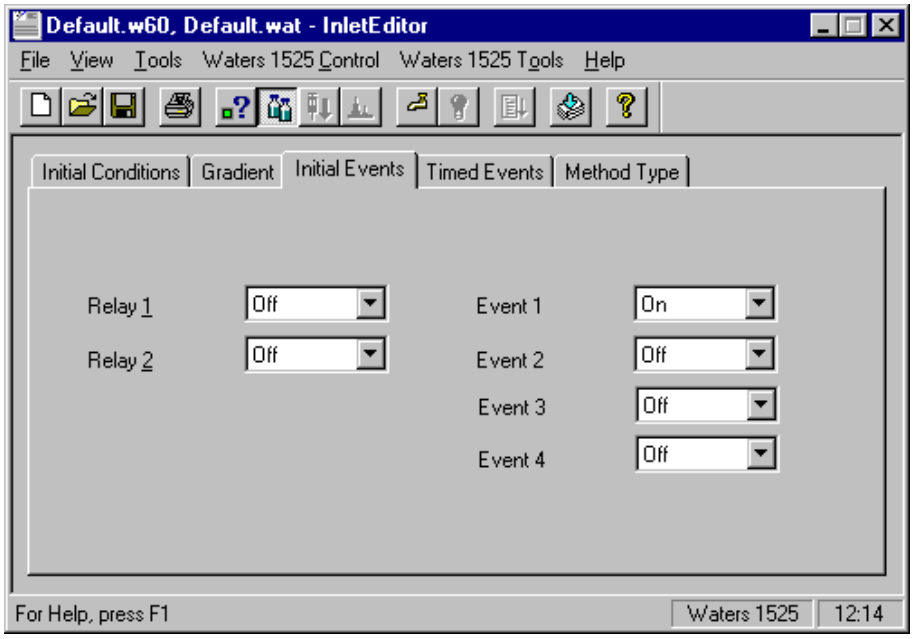


Figure 2.66 *Initial Events page*

The external events are triggered by four contact closures (relays) through output terminals, which are located at the back of the instrument.

Waters 515

Relays 1 and 2 From the drop down list box, select **ON** or **Off** to activate or deactivate the relay.

Events 1 to 4 From the drop down list box, select **ON** or **Off** to activate or deactivate the event.

Waters 1525

Relays 1 to 4 From the drop down list box, select **ON** or **Off** to activate or deactivate the relay.

Waters 515/1525 Timed Events Page

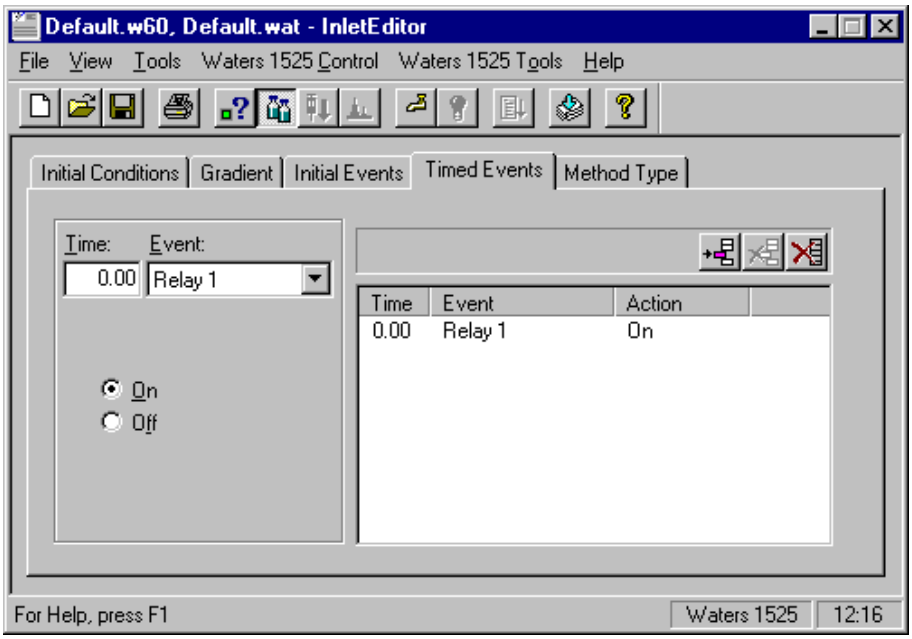


Figure 2.67 Timed Events page

Use the Event Table to program up to 16 events (both external and internal). Events can be triggered more than once and multiple events can be triggered simultaneously.

Time Enter the time (after injection) at which the event starts. Event rows are sorted automatically by time. **Note:** Different events can be programmed to occur at the same time. Range: 0.00 to 999.99 min.

Event Select an Event or Relay from the drop down list box.

Switch States

On Turns on a contact closure that triggers an external or internal event. With this function, the contact closure remains closed until an Off function is sent.

Off Turns off the contact closure for the event. With this function, the contact closure is broken.

Event Table Operation

To add an event, enter a time, event, action and value in the relevant boxes and press the  toolbar button. Note the first entry must have a time of 0.

To delete a single event, click with left mouse button on a time in the list and press the  toolbar button.

To delete all entries press the  toolbar button. This button is only available when there are entries in the timetable.

To modify an event, select the required entry in the timetable. The values will then be displayed in the edit boxes, and can be altered as appropriate. Once changed press  to re-enter the values into the timetable. If, however, you modify the time value such that it does not correspond to any existing entry in the timetable pressing  will result in a new entry being created in the timetable.

■ Waters 515/1525 Method Type Page

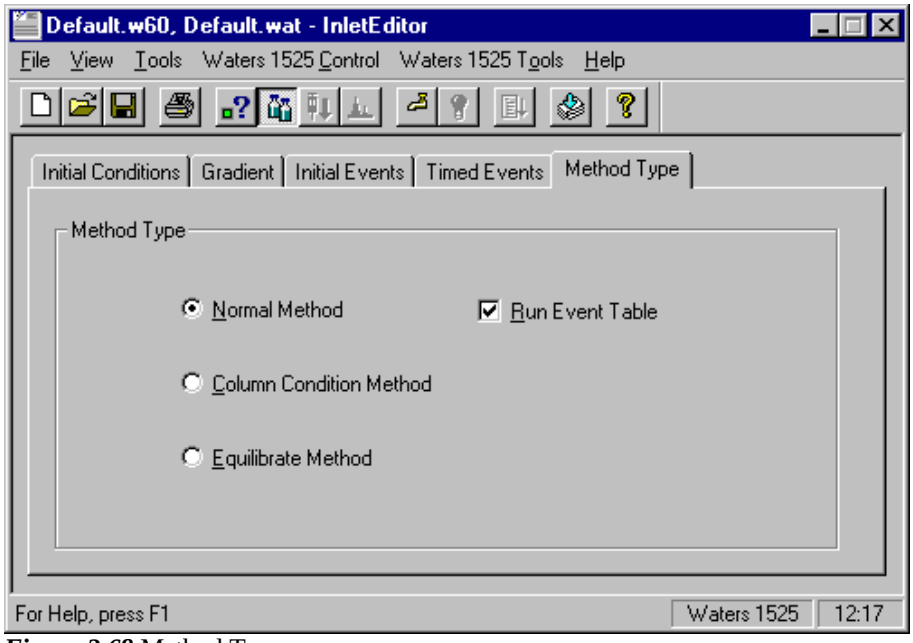


Figure 2.68 Method Type page

Method Type Specifies the type of method to create.

Normal Method The Method Type used for standard injections. Ensure that the Method Type is set to **Normal** unless you are performing one of the **procedures** listed below.

Column Condition Method Runs solvent through the column without injecting samples or running the Events table. Solvent is delivered using the gradient table specified in the Gradient page.

Equilibrate Method Delivers solvents and maintains solvent parameters using the values defined on the Initial Conditions page.

Run Event Table Check this box to run the table of timed events during the method. This option is only active if the **Normal** or **Column Condition Methods** are selected.

Notes

Notes

CE Instruments

Chapter 3

CE Instruments GC8000 Gas Chromatograph

On a CE Instruments GC8000, MassLynx can control the oven temperature, the injector zone temperatures, the valve times, the dump valve and 4 external event times.

To change GC Parameters

1. Choose **Set up Inlet** from the Acquisition Control Panel Instrument menu.

   - or -

   Double click on the picture of the GC on the Acquisition Control Panel to display the GC8000 inlet editor shown below.

2. Make any changes to the parameters. **Note:** The oven temperature ramp can be modified either by using the keyboard to enter times, temperatures and rates, or by dragging the small red handles on the graph with the mouse.

3. Save the method using either **Save** or **Save As** from the File menu.

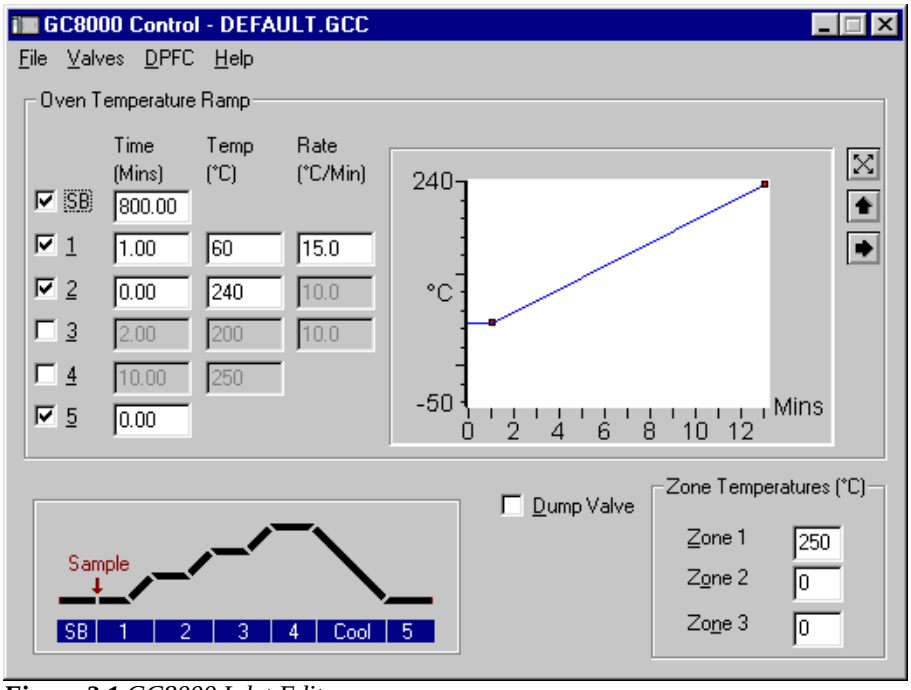


Figure 3.1 *GC8000 Inlet Editor*

The time and temperature range of the oven temperature ramp can be controlled using the buttons displayed to the right of the ramp. Clicking on  will increase the range shown on the time axis. Clicking on  will increase the range shown on the temperature axis. Clicking on  alters the display ranges so that the oven temperature display fills the graph.

A full description of all the parameters in this editor is given in the *GC8000 Series Instruction Manual*.

Changing Valve Event Times

Timed events such as Purge and Split times can be included in the GC method. These are programmed using the GC 8000 Valve Control editor shown below.

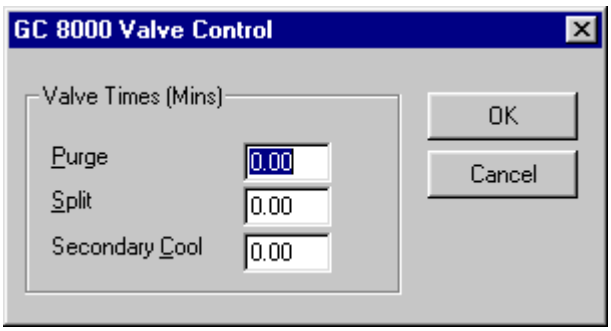


Figure 3.2 *GC8000 Valve Editor*

To display this dialog select **Valve Timetable** from the **Valves** menu. The events parameters are stored to disk when the GC parameters are saved, not when this dialog is closed so ensure that parameters are saved before starting an acquisition.

To control the GC8000 DPFC option

MassLynx can control the DPFC option on the GC8000 for Quattro II and Platform instruments.

1. Select **Configuration** from the GC8000 editor **DPFC** menu.

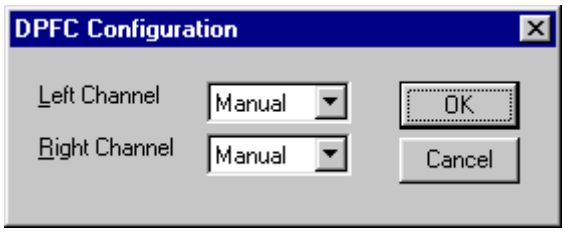


Figure 3.3 *DPFC Configuration dialog*

2. Configure the left and right channels as required. Each channel can be set to flow, pressure or off.

3. Select **Left Channel** or **Right Channel** from the GC8000 editor **DPFC** menu to load either the Flow Ramp or Pressure Ramp Editor depending how the channel is configured.

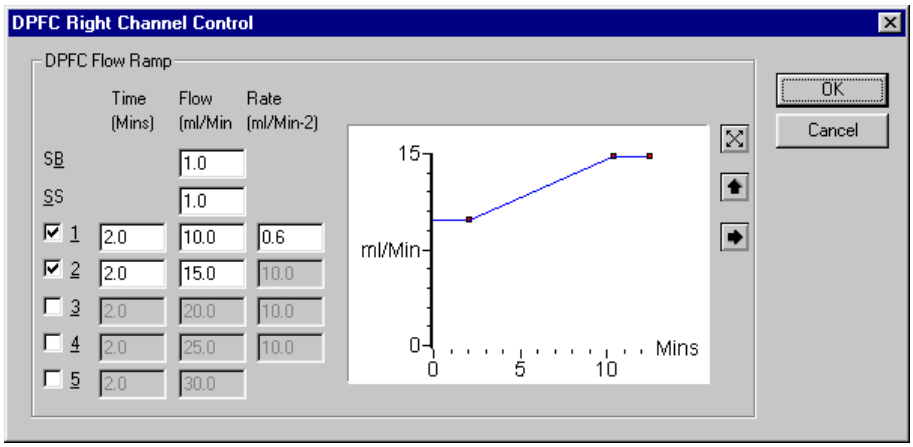


Figure 3.4 *DPFC Flow Ramp Editor*

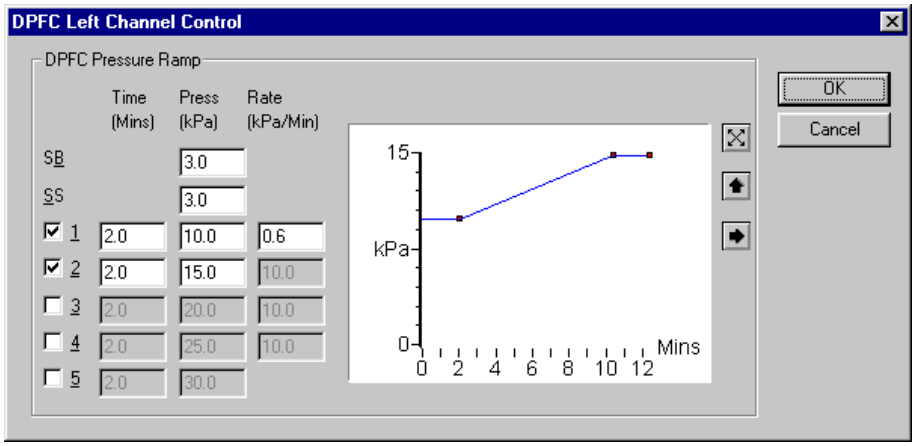


Figure 3.5 *DPFC Pressure Ramp Editor*

4. Make any changes required and press **OK** to exit and save changes.

CE Instruments AS800 Auto Injector

The CE Instruments AS800 Auto Injector can be used with the CE Instruments GC8000 gas chromatograph. The autosampler is programmed from MassLynx using the A200S editor. It is programmed in exactly the same way as the A200S system described above.

A full description of all the parameters in this editor is given in the *AS800 Autosampler Instruction Manual*.

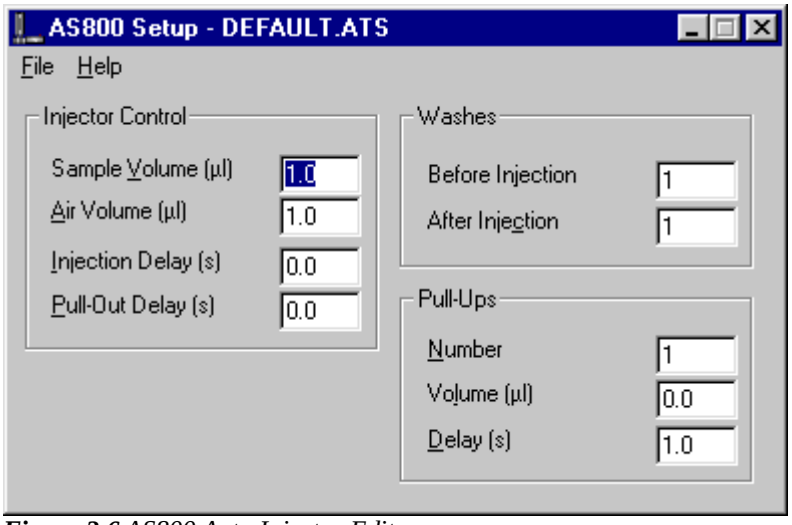


Figure 3.6 *AS800 Auto Injector Editor*

Notes

Notes

Gilson Systems

Chapter 4

Gilson Autosamplers

Introduction

- **Supported Models**

The Gilson Software can be used to control any of these models:

Gilson 215 Gilson 231XL

Gilson 232XL Gilson 233XL

Gilson 222XL

The Gilson 232XL and 233XL also require the Gilson 402 Dilutor. We also support the Gilson 401C Dilutor although this has now been discontinued by Gilson.

The Gilson 215 has a dilutor built in, but it does require a Gilson 819 Valve Actuator.

- **Setting up**

The first time MassLynx is run with a Gilson Autosampler it needs to know which autosampler is being used. The following dialog is displayed.

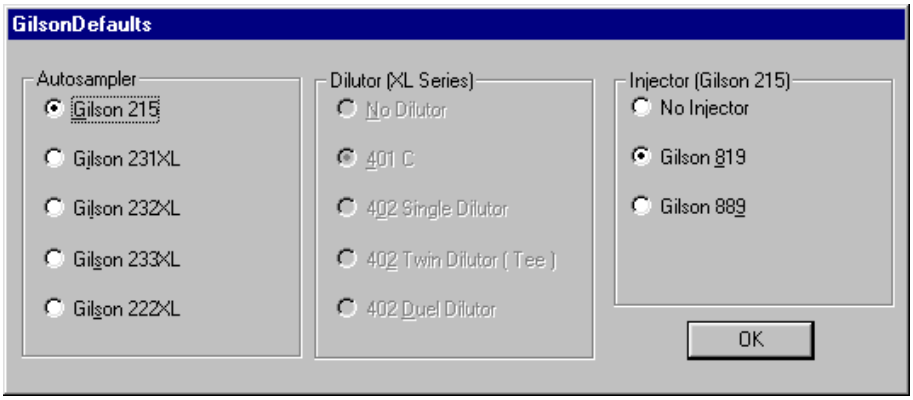


Figure 4.1 *Gilson Defaults dialog*

Select the Autosampler, Dilutor and Injector installed and press **OK**. **Note:** This only needs to be done the first time you use MassLynx or if the type of autosampler is changed.

The Gilson Toolbar

The Gilson toolbar has three extra buttons on it, which are:

Click	To
	Prime the Dilutor.
	Generate Custom Racks.

Gilson Configuration Pages

These pages contain information that is used to configure the autosampler. To access them press the  button or select **Gilson AutoSampler** from the **Inlet Editor View** menu.

The Gilson Task List

This page is used to build up a set of tasks into a method that is then used to perform the injection. The available tasks are contained in the **Task** drop down list box and the parameters displayed will depend on which task is selected.

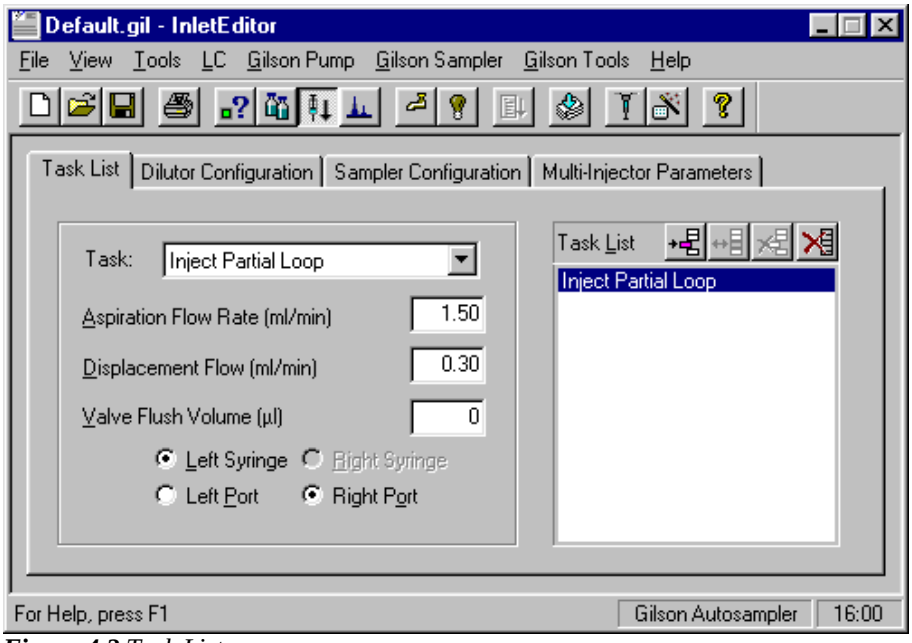


Figure 4.2 *Task List page*

Adding and Deleting Tasks (Gilson)

To add a task select it from the **Task** drop down list box, set the parameters and press the add  button. The task will be added to the end of the list.

To delete a single task, select it from the **Task List** and press the delete  button.

To clear all of the tasks in the Task List press the clear all  button.

Modifying Tasks (Gilson)

To modify a task select it from the **Task List**, change the required parameters and press the add  button.

Moving and Copying Tasks (Gilson)

To move a task, select it with the mouse, hold the mouse button down and move the task to the required position.

To copy a task follow the procedure for moving tasks but hold the **CTRL** key down when moving the mouse.

The Individual Tasks (Gilson)

This section contains tables listing the individual parameters for each task.

Inject Partial Loop

This is the main task that is used to inject. The Injection volume is entered in the sample list.

Parameter	Description
Aspiration Flow Rate	This is the flow rate at which the sample is drawn into the needle.
Displacement Flow	This is the flow rate at which the sample is injected into the loop.
Valve Flush Volume.	This is the volume of solvent that is flushed through the valve after the injection. It is displaced at the Displacement flow.

Table 4.1 *Inject partial loop parameters*

Detailed below is a list of the steps that occur during the inject partial loop task.

Steps:

1. Move to vial
2. Aspirate air gap if required
3. Move Zarm down to vial depth
4. Aspirate injection volume + injection flush volume
5. Move Zarm back to travel height
6. Move to injection port
7. Move to injection depth
8. Switch valve to inject position
9. Dispense injection flush volume
10. Switch valve to load
11. Dispense injection volume
12. Switch valve to inject
13. Pulse output contact
14. Dispense air gap
15. Rinse valve if a flush volume has been specified

Note: The Left and right valve become enabled when using a Gilson 233XL.

Rinse Injection Port

This task is used to rinse the injection port with solvent from the reservoir.

Parameter	Description
Rinsing Volume	This is the volume of solvent that is to be rinsed through the needle.
Displacement Flow	This is the flow rate at which the solvent is injected into the valve.

Table 4.2 *Rinse Injection Port parameters*

Note: The Left and right valve become enabled when using a Gilson 233XL.

Rinse Inside Needle

This task is used to rinse the inside of the needle with solvent from the reservoir.

Parameter	Description
Rinsing Volume	This is the volume of solvent that is to be rinsed through the needle.
Displacement Flow	This is the flow rate at which the solvent is rinsed through the needle.
Rinse Station	This is the rinse station at which you would like the rinse to take place. If this is set to auto then the nearest rinse station is chosen.

Table 4.3 *Rinse Inside Needle parameters*

Rinse Outside Needle

This task is used to rinse the outside of the needle with solvent from the reservoir.

Parameter	Description
Rinsing Volume	This is the volume of solvent that is to be rinsed through the needle.
Displacement Flow	This is the flow rate at which the solvent is rinsed through the needle.
Depth	This is set to the depth that the needle should move to for rinsing.
Rinse Station	This is the rinse station at which you would like the rinse to take place. If this is set to auto then the nearest rinse station is chosen.

Table 4.4 *Rinse Outside Needle parameters*

Because this task dispenses the solvent through the inside of the needle it also acts as a rinse inside needle.

Note: Rinsing the Outside of the needle is not available on the Gilson215

Set Electrical Contact

This task is used when you would like to set one of the output contacts.

Parameter	Description
Contact Number	This is the number of the contact that you would like to set.
State	This is the state that you want to set. Open, Close or Pulse.

Table 4.5 *Set Electrical Contact parameters*

Wait For Contact

This task is used when you need to wait for a contact state.

Parameter	Description
Contact Number	This is the number of the contact that you would like to set.
State	This is the state that you want to set. Open, Close or Pulse.

Table 4.6 *Wait For contact parameters*

Wait For Time

This task is used if you need the machine to wait for a specified time.

Parameter	Description
Time	The time that you wish to wait for.

Table 4.7 *Wait For Time parameters*

- **Gilson Dilutor Configuration Page**

This page is used to set parameters specific to the Dilutor.

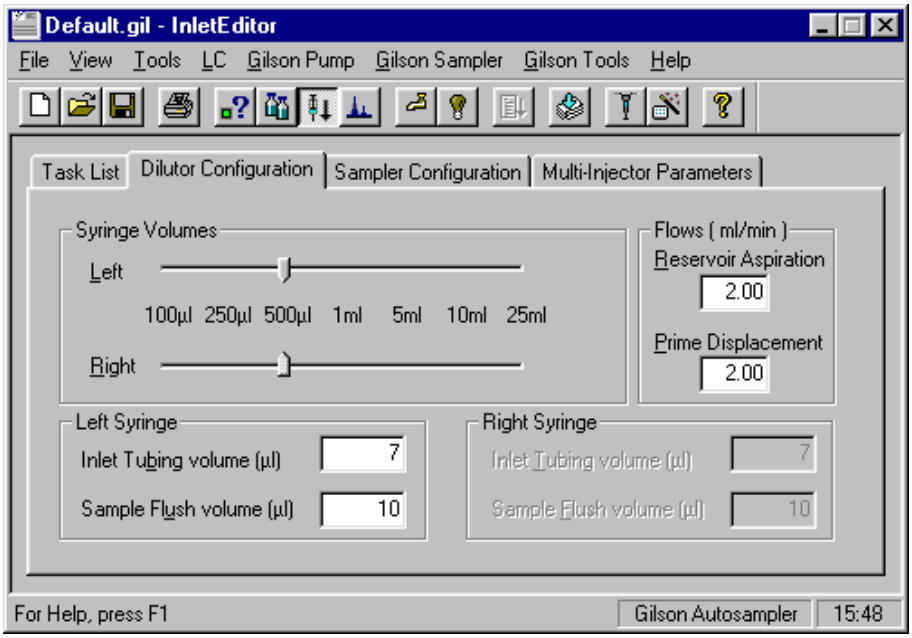


Figure 4.3 *Dilutor Configuration page*

Syringe Volumes The size of the currently installed Left and Right syringes.

Reservoir Aspiration Flow This is the flow rate at which solvent is drawn from the reservoir (the default value is usually sufficient).

Prime Displacement Flow This is the flow rate at which the solvent is displaced during the prime dilutor (the default value is usually sufficient).

Inlet Tubing volume This is the volume of the tubing between the injection port and the rheodyne valve. It is the volume of air used to push the sample through into the injection loop.

Sample Flush volume This is the amount of sample that is drawn with the injection valve. This amount is then injected before the valve switches to fill the tube between the valve and the injection port. Any excess will go to waste.

Note: When using the Gilson 402 Dilutor, the Left and Right syringe radio buttons are enabled allowing you to use the left and right syringes. This is not yet available.

Gilson Sampler Configuration Page

This page is used to set parameters specific to the Sampler.

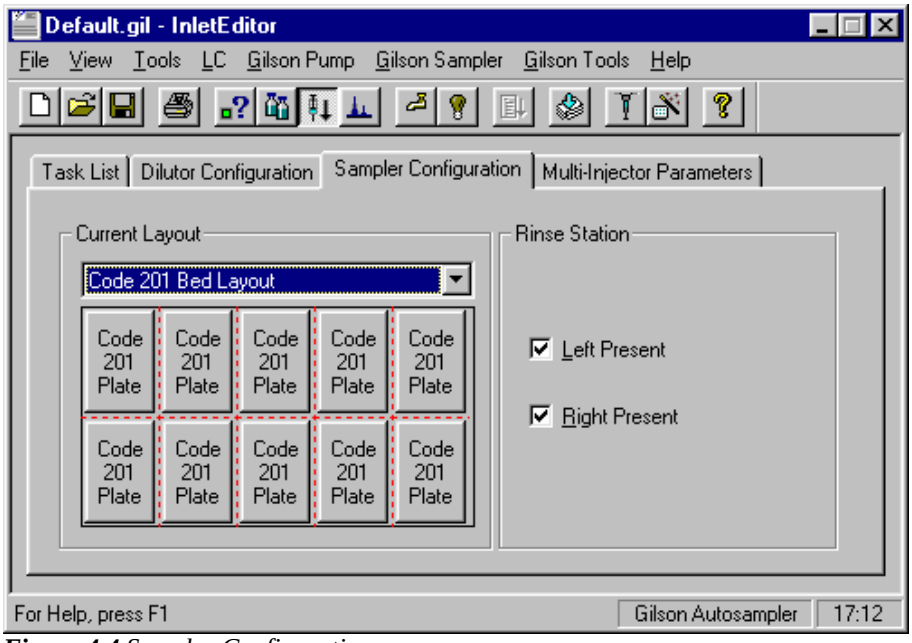


Figure 4.4 *Sampler Configuration page*

Current Layout Select the required layout from the drop down list box. A picture of the selected bed layout is displayed below the name.

Rinse Stations Present Check the boxes if the rinse stations are present. Left and right are as you look at the machine.

Note: When using the Gilson 215 the right rinse station will be disabled.

Gilson Multi-Injector Parameters Page

This page is used to set parameters specific to the Gilson Multi-Injector System. This is an autosampler device that injects up to 8 samples simultaneously. The Multi-Injector itself consists of a Gilson 215 autosampler in conjunction with a Gilson 889 multi-valve injector. The device has eight needles connected to the robot arm and a syringe for each needle. The geometry of the autosampler is designed so that the 8 needles will enter 8 separate wells of a microtitre plate. The 8 samples are picked up at the same time and then deposited into 8 separate injection loops. The valves connected to these loops can then be controlled individually so that each of the samples can be sent to the mass spectrometer at any specified times.

To enable these parameters the following configuration must be defined.

1. Select **Advanced Configuration** from the **Gilson Sampler** menu.
2. On the **Hardware** tab select **Gilson 215** from the **Sampler** drop down list box.
3. On the **Hardware** tab select **Gilson 889** from the **Valve** drop down list box.
4. On the **Hardware** tab select **All samples to same file** from the **Multi-Injector Mode** drop down list box.
5. On the **Hardware** tab check the **Enable Inject Ahead** box.
6. Press **OK**.

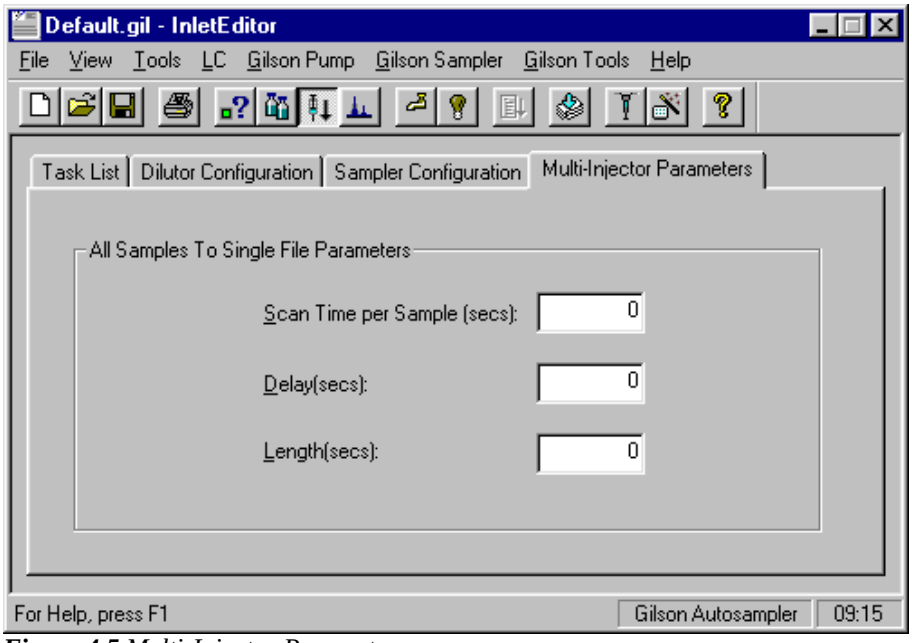


Figure 4.5 *Multi-Injector Parameters page*

Scan Time per Sample This defines the analysis time spent on each sample.

Delay This is the time for the sample to travel from the injection port to the mass spectrometer.

Length This is the amount (in seconds) of the chromatogram that is used to create the data files for each of the samples.

Gilson Multi-Injector Processing

A complete row of 8 samples are collected simultaneously and placed in the injection ports. The injection valve for the first sample is switched to inject and a contact closure is used to signal the mass spectrometer to initiate scanning. Each subsequent sample is then injected every *T* seconds, where *T* is the *Scan Time Per Sample* defined on the multi-injector parameters page. Once all 8 samples have been injected the next set of samples are loaded in the injection loops. The first of these samples is injected after a time *T* from the last sample of the previous row.

The scanning time defined in the Mass Spectrometer method should be long enough so that all the samples can be injected and scanned. This time has to be calculated by the user.

Data for all samples is written to one file, the BatchDataFile, see **Figure 4.6**. Each peak within this chromatogram relates to a separate sample.

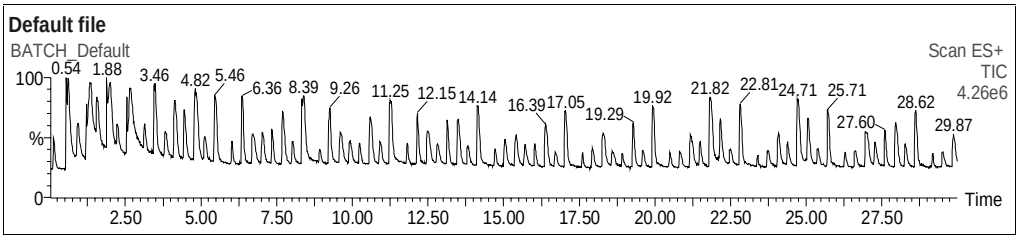


Figure 4.6 *Multi-Injector Batch File*

The file name of the BatchDataFile is either based on the sample list name or the OpenLynx Job ID. A prefix of BATCH_ is added to this name so that it can be recognised as a BatchDataFile. E.g. for a sample list called *Test.SPL*, the name of the BatchDataFile will be *BATCH_Test.RAW*.

Once the scanning for the BatchDataFile is complete ChroSplit.exe is used to create individual data files for each sample in the batch. ChroSplit.exe should be defined in the Acquire Process column for the first sample in the sample list or on the OpenLynx Setup Acquisition Process page.

ChroSplit reads the BatchDataFile.RAW and splits it into individual files based on the values defined on the Multi-Injector Parameters page. It ignores the first part of the file that is the **Delay**. The rest of the file is split into **Scan Time per Sample** sections and the scans acquired from the start of each of these sections for the defined **Length** are copied into the individual data files.

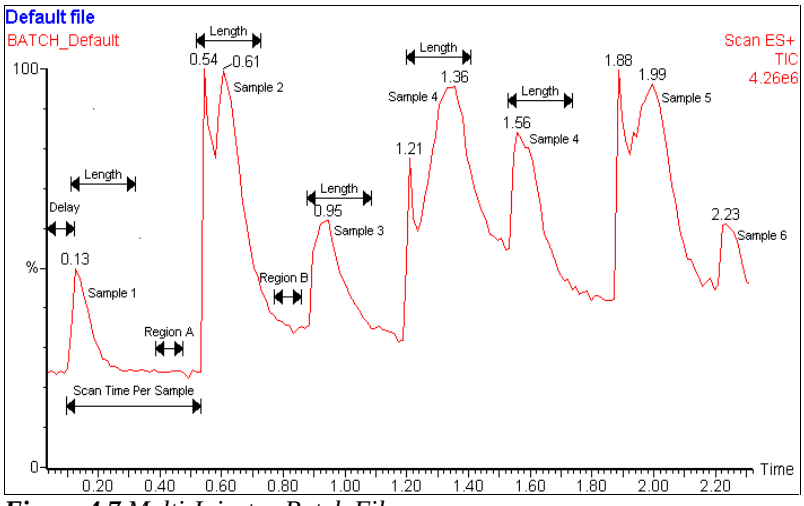


Figure 4.7 *Multi-Injector Batch File*

Some of the scans between any two samples will contain some mixing of samples (e.g. Region B in **Figure 4.7**) or not contain data relating to either sample (e.g. Region A in **Figure 4.7**). The data in these regions is not required, therefore only data in Length region is copied.

Once all data files have been created by ChroSplit the acquisition will proceed with any processing defined in the Process column for the first sample in the batch. For all subsequent samples in the batch no data is acquired only the processes are initiated.

ChroSplit currently writes two data files per sample. The first has a re-normalised retention time so that the retention time of the first scan for each sample is set to 0. This allows analysis of the masses to proceed via loop injection, which simply searches for masses contained within the scan at a user-defined retention time. The other file written retains its original retention time and is used to assess the accuracy of the ChroSplit procedure. This second data file has the prefix "CHECK_" added to the .RAW file name.

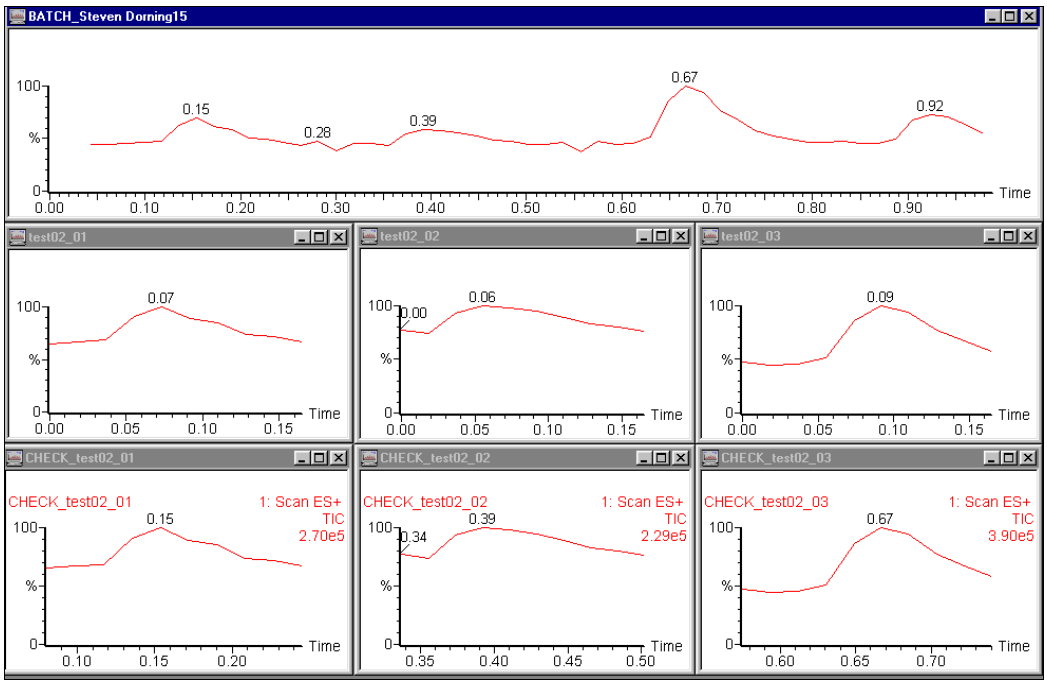


Figure 4.8 *The results of using ChroSpilt.exe. Upper shows the Batch file, middle the re-normalised files and lower the check files*

Problems with ChroSplit

If ChroSplit fails to copy the BatchDataFile scans correctly (due to an incorrect delay being defined or experimental faults, e.g. a change in pumping speed) then the delay and length parameters can be changed and the BatchDataFile reprocessed.

To do this the values in the timefile.tfl need to be changed. This file contains the time each sample reaches the mass spectrometer and is stored in the BatchDataFile.RAW directory. Also written to this file are the sample number, sample location for each sample and the multi-injector length and delay parameters.

```
[timefile]
MasterRawFile=Batch_xxxxx
Delay=4.5
Length=15
[Sample]  [Location]  [Injection Time]  [Sample ID]
1         "1,A"       0.195375         "Not used"
2         "1,B"       26.472376        "Not used"
3         "1,C"       46.591373        "Not used"
4         "1,D"       66.700378        "Not used"
```

Figure 4.9 *Example timefile.tfl*

1. Open the **timefile.tfl** using a text editor, change the **Delay** or **Length** as required and save the file.

2. Open the Sample List and change the Process for the first sample to ChroSplit.exe.

3. Press the  button to display the **Start Sample List Run** dialog.

4. Ensure that only the **Auto Process Samples** box is checked, the **Run From Sample** = 1 and the **Run To Sample** = 1, then press **OK**.

5. This will split the BatchDataFile into the individual *.RAW files.

6. On the Sample List change the Process back to the original *processname* and repeat step 3.

7. Ensure that only the **Auto Process Samples** box is checked, the **Run From Sample** = 1 and the **Run To Sample** = *last sample in the list*, then press **OK**.

The data file for each sample will be recreated overwriting the previous files.

See the OpenLynx Users Guide, Introduction chapter for details on importing OpenLynx Batch files into the Sample List.

Gilson Advanced Options

Gilson Tray Options

To display the Tray Options dialog, select **Options** from the **Gilson Tools** menu on the Inlet Editor.

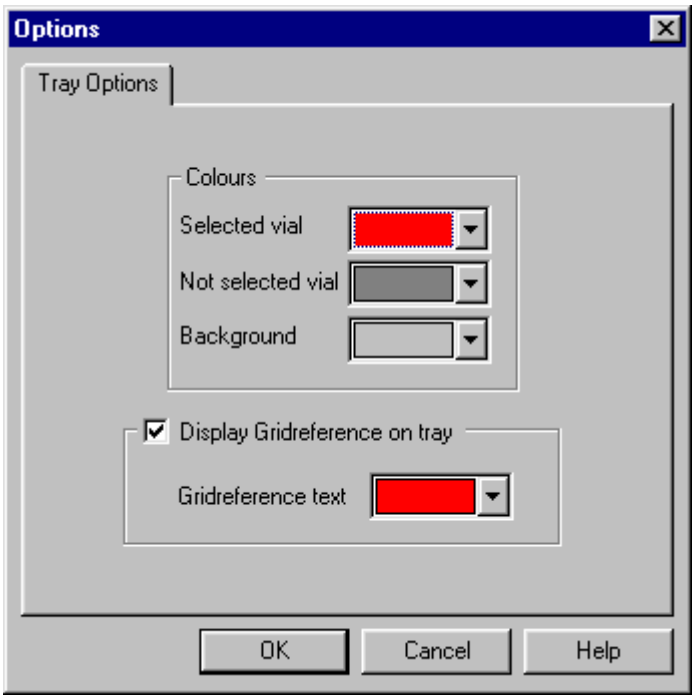


Figure 4.10 *Tray Options dialog*

Colours Select the colour to display the **Selected vial**, **Non selected vial** and **Background** from the appropriate drop down list box.

Display Gridreference on tray Check this box to display the grid reference on the tray.

Gridreference text From the drop down list box, select the colour in which you want the grid reference text to be displayed.

Gilson Plate Generator

To display the Custom Rack Generator dialog, select **Plate Generator** from the **Gilson Tools** menu on the Inlet Editor dialog or press the  button.

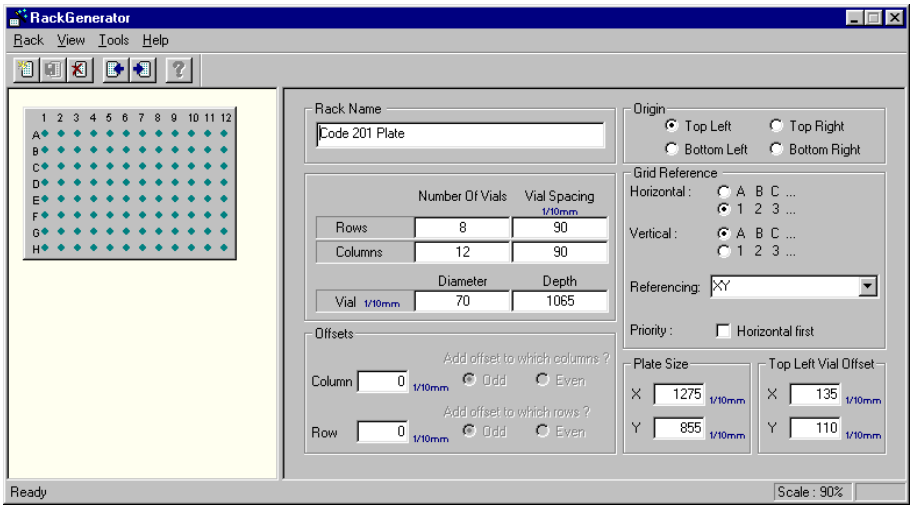


Figure 4.11 *Custom Rack Generator*

Rack Name The name of the plate that is currently being edited.

Origin The corner of the rack that the vial grid referencing starts from.

Rows The number of vials in a row and the distance between each center.

Columns The number of vials in a column and the distance between each center.

Vial Diameter does not affect any parameters apart from how the tray looks in the Rack Generator. Depth affects how deep the needle travels into each vial when sampling. Decreasing the depth value will make the needle travel down further into the vial.

This control is very important. An incorrect setting could send the needle through the bed and bend it.

Grid Reference Allows the user to select the way that the vial rows and columns are referenced, e.g. whether the rows are alphabetical or numerical.

Referencing This has three options

- XY which references the vials A1, B1 etc.
- Sequential Discontinuous which numbers the vials 1, 2, 3 across a row, left to right, and then starts the next row from the left again.
- Sequential Continuous which numbers the vials 1, 2, 3 across a row, left to right, then continues number the next row, right to left etc.

If the Gilson autosampler is used with OpenLynx then the vial referencing must be set to either sequential continuous or sequential discontinuous.

Priority Check the **Horizontal First** box if samples are to be acquired horizontally across the plate.

If Referencing = X,Y, Horizontal = Letter, Vertical = Number and Horizontal Priority is checked, this will result in samples being acquired in the order A1, A2, A3. If the Horizontal Priority box is not checked samples will be acquired in the order 1A, 1B, 1C etc.

If Referencing = sequential continuous or discontinuous and Horizontal Priority is checked, this will result in samples being acquired from row 1 then row 2. If the Horizontal Priority box is not checked samples will be acquired from column 1 then column 2 etc.

Offsets Allows alternate vial rows or columns to be offset.

Plate Size The size of the plate to its outside edges.

Top Left Vial Offset The measurement to the center of the first vial from the top left corner of the plate.

Creating and Deleting Plates (Gilson)

To create a new rack press the  button. A new default rack is displayed, change the **Rack Name**, enter the appropriate values and press the save  button or select **Save Current Rack** from the **Rack** menu. New racks are saved to the MassLynx **Plates** directory.

To copy a custom rack, page through the list of saved custom racks using the  and  toolbar buttons. The **Previous Rack** and **Next Rack** options on the **Rack** menu perform the same operation. When the required rack is displayed change the **Rack Name**, enter the appropriate values and press the save  button or select **Save Current Rack** from the **Rack** menu. New racks are saved to the MassLynx **Plates** directory.

To delete a custom rack select the rack to delete, by typing the name in the **Rack Name** box or by paging through as above, and press the delete  button or choose **Delete Current Rack** from the **Rack** menu.

Note: All of the spacings and the **vial section** are stored in 0.1 mm units.

Note: When defining a custom plate for use with a multi-injector the plate is required to be compatible with the position of the 8 needles of the autosampler.

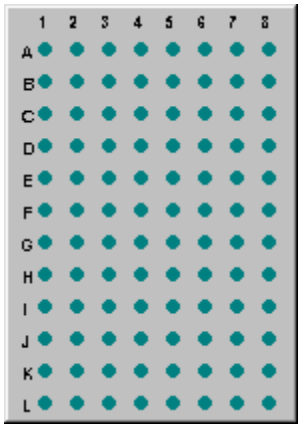
- The Plate must have eight columns.
- The position of the vials should allow all eight needles to enter a separate vial.
- There should be no odd or even offsets for any of the vial positions.

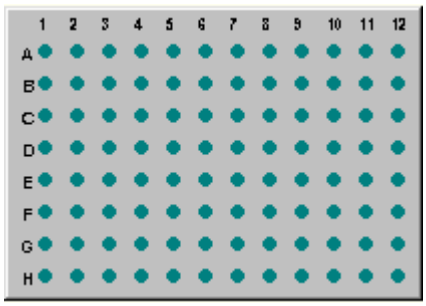
Default Plate Settings (Gilson)

Selecting **Default Settings for New Rack** from the **Tools** menu displays the **Default Settings** dialog. This dialog allows the default settings used when creating a new rack to be defined. Field descriptions are the same as above.

Rotating and Scaling Plates (Gilson)

Selecting **Rotate Rack** from the **View** menu will rotate a rack by 90 degrees. For example:





Selecting **Scale Rack** from the **View** menu displays the following dialog.

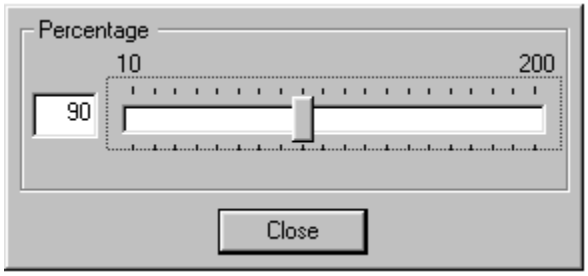


Figure 4.12 *Scale Rack dialog*

Move the slider or enter a new value to change the size of the rack as displayed in the Plate Generator dialog.

The Gilson Bed Layout Editor

To display the Bed Layout Editor dialog, select **Bed Layout Editor** from the **Gilson Tools** menu on the **Inlet Editor** dialog.

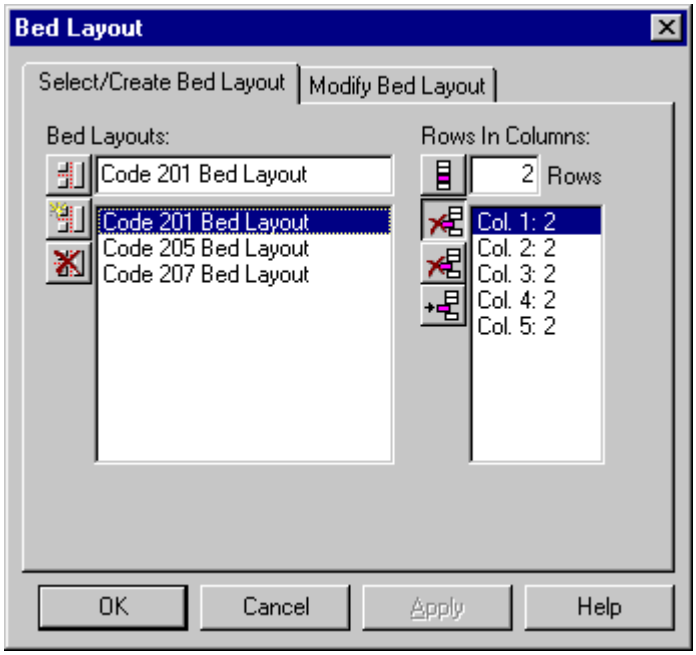


Figure 4.13 *Bed Layout Dialog*

To Create a New Bed Layout (Gilson)

1. Highlight a bed layout similar to the one you want to create and press the  button to create a new layout. The layout appears in the **Bed Layouts** list as the same name with a 1 at the end, e.g. Code 201 Bed Layout1.

2. To change the name of the layout, type the new name into the Bed Layouts text box and press the  button. The name is updated in the Bed Layouts list box.

New bed layouts are saved to the MassLynx **Racks** directory.

To Delete a Bed Layout (Gilson)

1. Highlight a bed layout you wish to delete and press the  button. A dialog box will ask you to confirm the deletion. Press the **OK** button to delete the bed layout.

Modifying the Number of Rows and Columns (Gilson)

To change the number of rows in the current column, type the new number into the **Rows** box and press the  button.

To append a new column, press the  button.

To delete the current column press the  button.

To insert a column, click on the column before which you want to insert and press the  button. **Note:** The column inserted will have the same number of rows as the column highlighted.

Modify Bed Layout (Gilson)

If the plate position or type needs changing select the **Modify Bed Layout** tab.

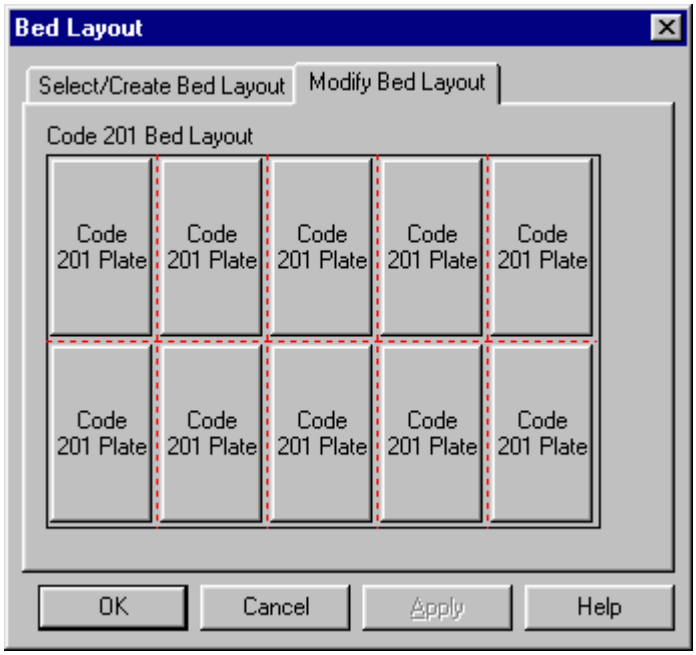


Figure 4.14 *Modify Bed Layout Dialog*

Click on one of the code plates to display the **Plate Position and Type** dialog.

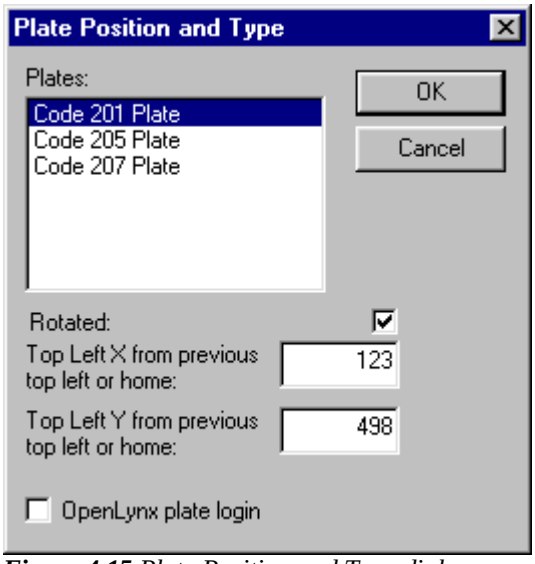


Figure 4.15 *Plate Position and Type dialog*

This dialog allows you to select a new plate from a list of possible options, and change its actual position on the bed. Measurements for plate positions are always taken from the top left corner of each plate. The X value is the measurement from the currently selected plate to the plate immediately to the left. The Y value is the measurement from the currently selected plate to the plate immediately above. If there is no plate, to the left or above, then measurements are taken from the Home position, which is where the needle sits when not in use.

Rotated Check this box if the plate is rotated.

OpenLynx plate login If this box is checked and **Use current MassLynx autosampler bed layout** is checked in the OpenLynx Manager program, then the plate at this position can only be used for plate login on the OpenLynx Login program.

Adjusting The Arm Height on a Gilson 215

The first time the Gilson software configuration pages are accessed the following dialog will be displayed. Type in the **Needle Height** that you have set the Gilson to and press **OK**.

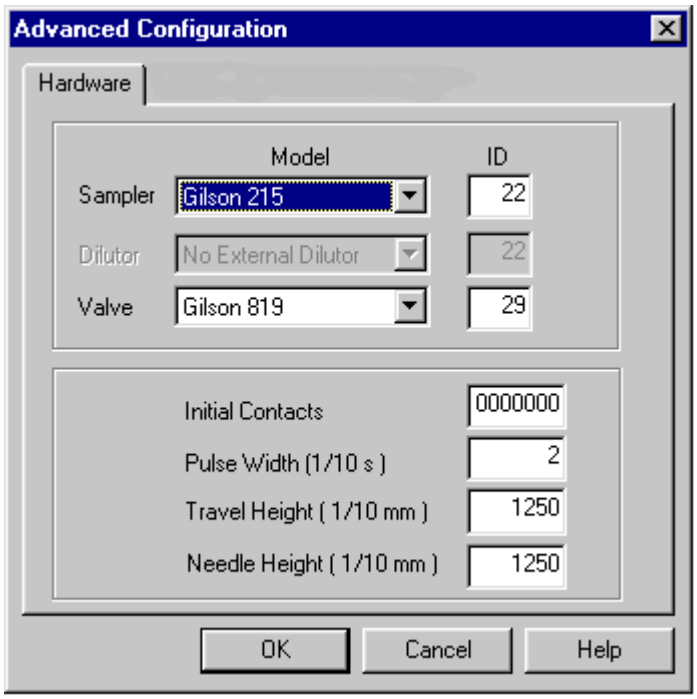


Figure 4.16 *Injection Parameters dialog.*

Other Advanced Options (Gilson)

The advanced options dialogs can be accessed by choosing **Advanced Configuration** from the **Gilson Sampler** menu option on the Gilson AutoSampler dialog.

The parameters on these pages will be set up at installation and should not need changing.

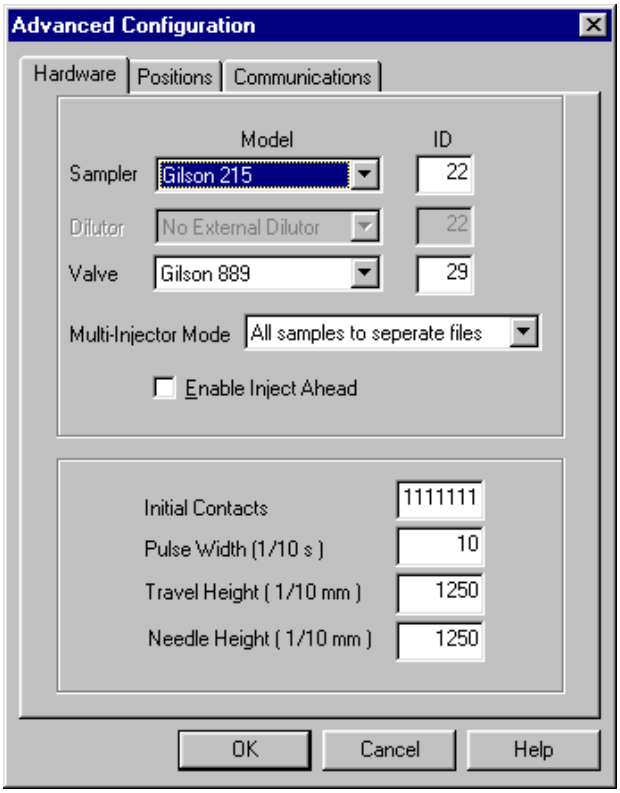


Figure 4.17 *Hardware Configuration Dialog*

This page defines the type of Gilson AutoSampler, Dilutor and Valve used. It also shows the state of the initial electrical contacts to the AutoSampler and pump, the pulse width and needle parameters.

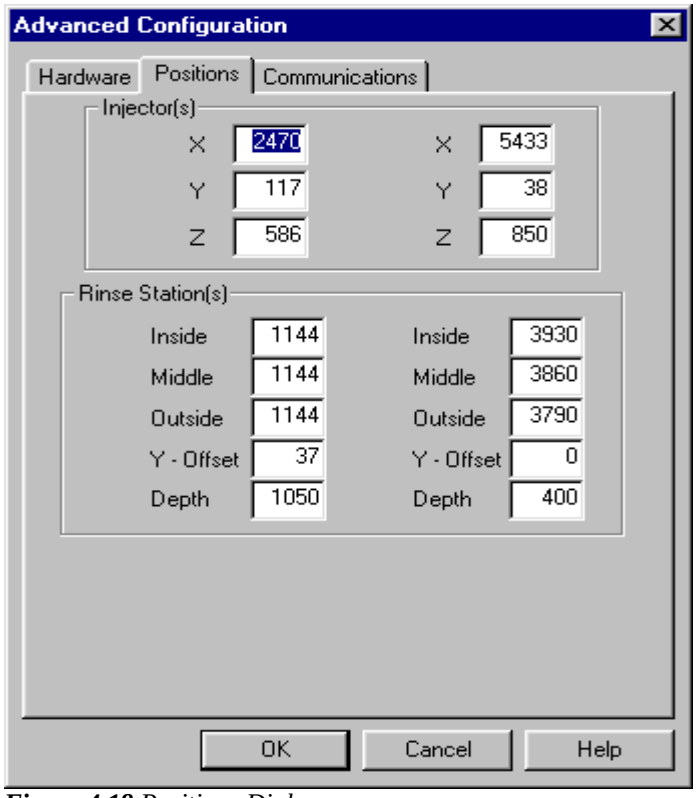


Figure 4.18 *Positions Dialog*

This page defines the integer position from the Home position of the needle, i.e. the position of the needle when not in use. It also defines the distances the needle needs to travel to the rinse stations.

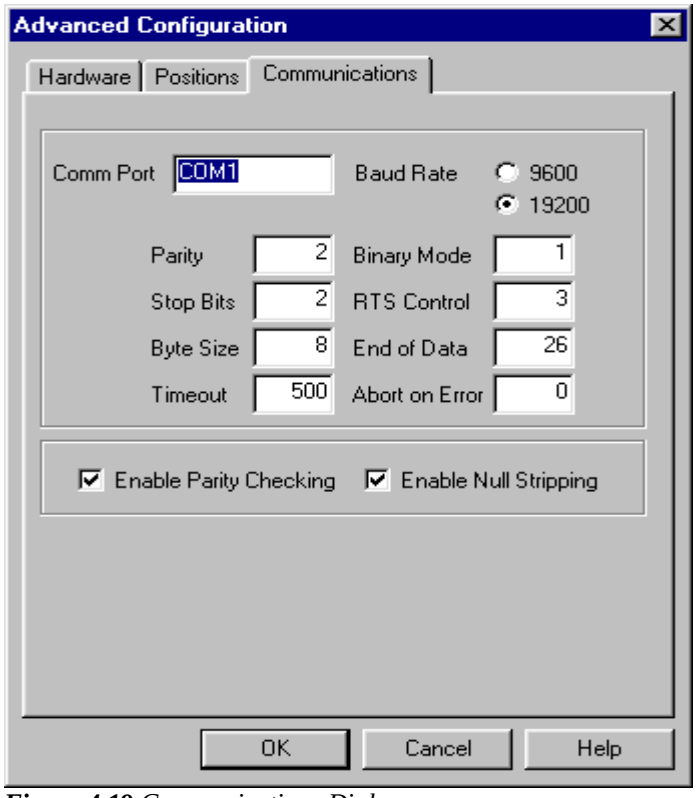


Figure 4.19 *Communications Dialog*

This page defines the serial line communication between the Gilson and the PC.

Gilson Pump

The Gilson Pump pages can be accessed by selecting **Gilson Pump** from the **View** menu on the Inlet Editor or by pressing the  toolbar button.

- **Gilson Solvents and Flows Page**

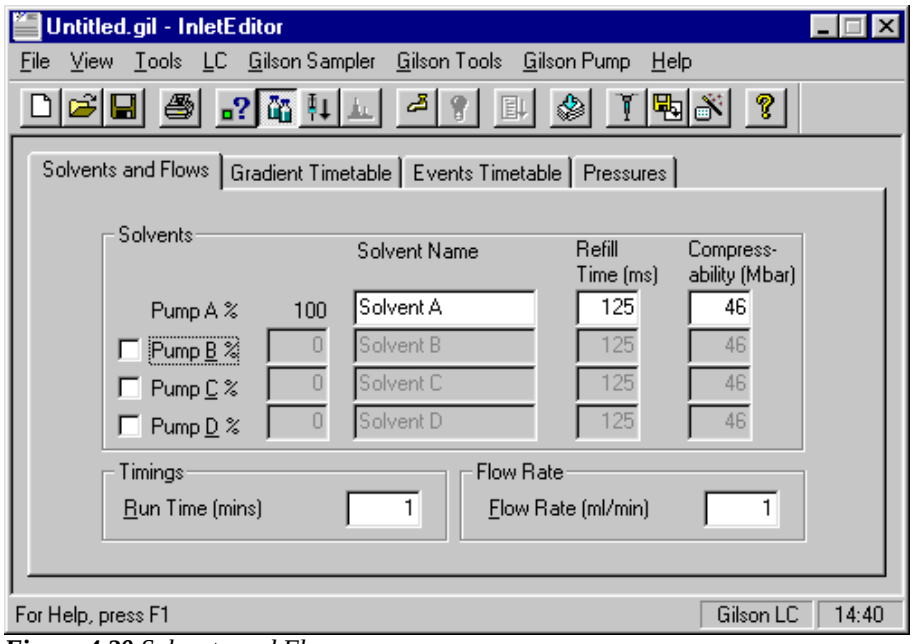


Figure 4.20 *Solvents and Flows page*

Solvents Up to four solvents will be displayed depending upon the system configuration. The total value of all the solvent percentages added together must not exceed 100%.

Pump A This is the remainder percentage after the solvent percentages have been set for the other pumps.

Pump B, C, D These can either be enabled or disabled by checking the box next to the individual pumps. The values can be set to the required percentage of flow delivery.

Solvent Name Type in the solvent name.

Refill Time This is the time required for the piston return stroke. Normally it is set to the lowest value (125ms). If cavitation or degassing occurs, then a higher value must be used. The minimum value is 125ms and the maximum 1000ms.

Compressibility This is used to calculate a flow rate compensation for the compressibility of the solvent. See the Gilson User Guide for suitable values.

Run Time This is the length of time, in minutes, the pump should run for.

Flow Rate This is the total flow rate of the solvent channels according to how you have configured the instrument.

Gilson Gradient Timetable Page

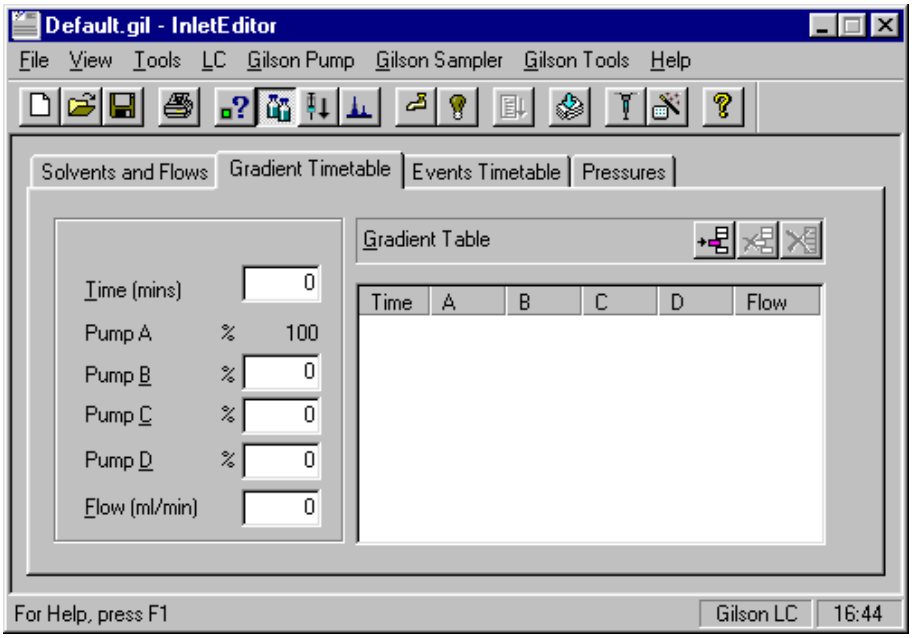


Figure 4.21 *Gradient Timetable page*

This page allows a gradient to be entered and edited. To operate in isocratic mode ensure that the timetable is empty.

To add a gradient, type in a time, the required percentages and the flow rate, in the relevant boxes and press the toolbar button. **Note:** The first entry must have a time of 0.

To delete a single gradient click with left mouse button on a time in the list and press the toolbar button.

To delete all entries press the toolbar button. This button is only available when there are entries in the timetable.

To modify a gradient, select the required entry in the timetable. The values will then be displayed in the edit boxes above the timetable, and can be altered as appropriate. Once changed press to re-enter the values into the timetable. If, however, you modify the time value such that it does not correspond to any existing entry in the timetable pressing will result in a new entry being created in the timetable.

Gilson Events Timetable Page

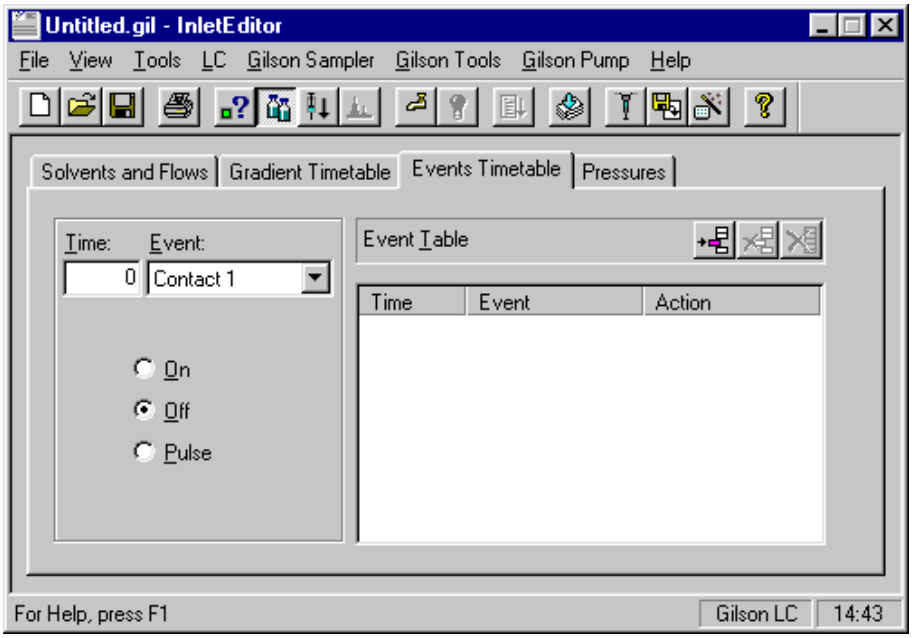


Figure 4.22 *Events Timetable page*

To add an event, enter a time, select an event from drop down box and press the  toolbar button.

To delete a single event, click with left mouse button on a time in the list and press the  toolbar button.

To delete all entries press the  toolbar button.

To modify an event, select the required entry in the timetable. The values will then be displayed in the edit boxes above the timetable, and can be altered as appropriate. Once changed press  to re-enter the values into the timetable. If, however, you modify the time value such that it does not correspond to any existing entry in the timetable pressing  will result in a new entry being created in the timetable.

- **Gilson Pressures Page**

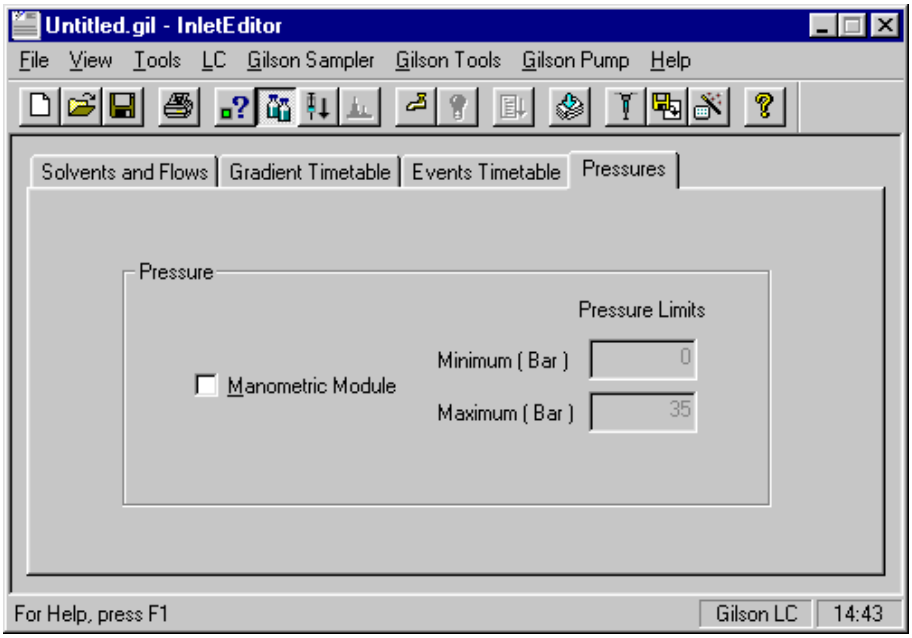


Figure 4.23 *Pressures page*

To set pressure limits check the **Manometric Module** box and enter a **Minimum** and **Maximum** pressure.

The maximum pressure limit is determined by the smallest pumphead size.

Pump Configuration

To change the number of pumps used select **Pump Configuration** from the **Gilson Pump** menu.

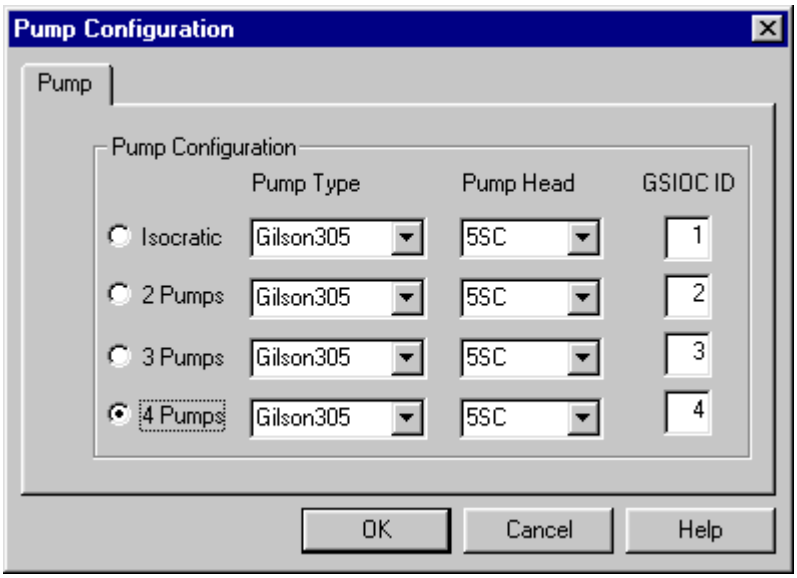


Figure 4.24 *Pump Configuration dialog*

Select the number of pumps, the pump type, pump head and the GSIOC ID (Gilson Serial Input Output Channel) required.

Notes

Notes

Hewlett Packard Systems

Chapter 5

Hewlett Packard 5890 Gas Chromatograph

Both the HP5890 Series I and Series II can be controlled by MassLynx. For the Series II instrument it is necessary to configure the GC to respond to Series I commands by setting a jumper in the GC. Your installation engineer will have done this. Before starting to use the GC the software must be configured to reflect the GC equipment in use e.g. the number of injectors and detectors etc.

To change GC Parameters (Hewlett Packard 5890 Gas Chromatograph)

1. Choose **Set up Inlet** from the Acquisition Control Panel Instrument menu

   or

   Double click on the picture of the GC on the Acquisition Control Panel to bring up the HP5890 inlet editor shown below.

2. Make any changes to the parameters. **Note:** The oven temperature ramp can be modified either by using the keyboard to type in times, temperatures and rates, or by dragging the small red handles on the graph itself using the mouse.

3. Save the method using either **Save** or **Save As** from the File menu.

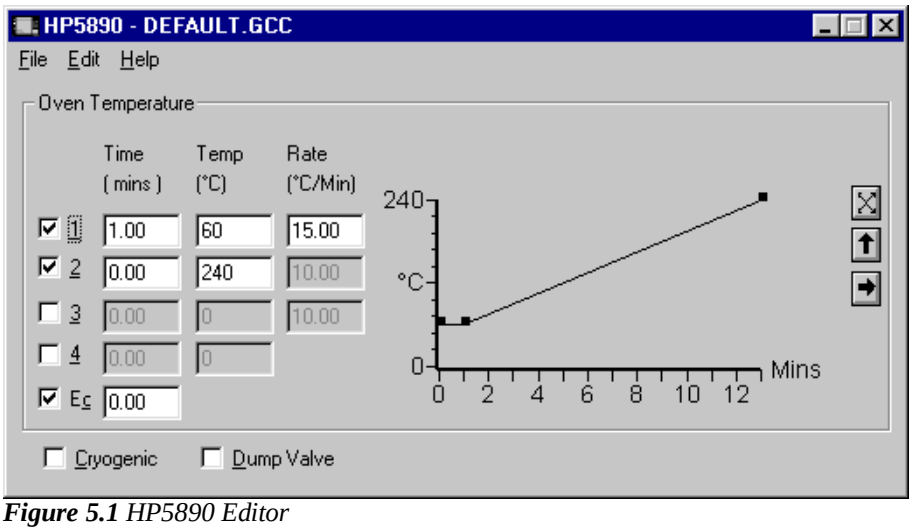


Figure 5.1 *HP5890 Editor*

The time and temperature range of the oven temperature ramp can be controlled using the buttons that appear to the right of the ramp. Clicking on  will increase the range shown on the time axis, clicking on  will increase the range shown on the temperature axis. Clicking on  alters the display ranges so that the oven temperature display fills the graph.

A full description of all the parameters in this editor is given in the *HP5890 Gas Chromatograph Reference Manual*.

- **To Change GC Configuration (Hewlett Packard 5890 Gas Chromatograph)**

1. Choose **Configuration** from the HP5890 Edit menu to display the configuration editor shown below.

2. Make any changes to the parameters.

3. Press **OK**. The parameters will be saved with the GC method when either **Save** or **Save As** is selected from the HP5890 File menu. Buttons in the HP5890 **Edit** menu that are not appropriate for the selected configuration will be grayed out.

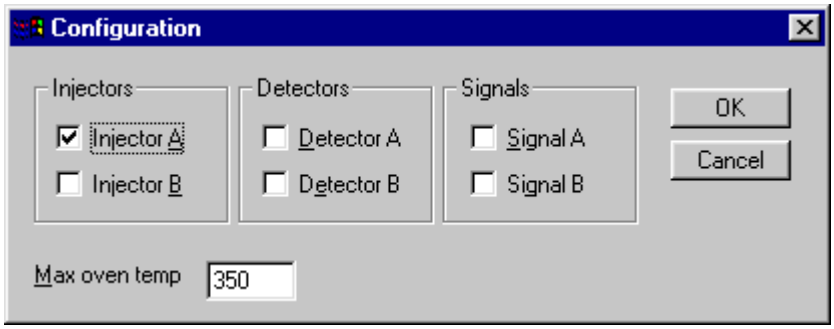


Figure 5.2 *HP5890 Configuration Editor*

The main HP5890 editor is used to set up the GC oven temperature program and to control the dump valve and cryogenic cooling options if fitted.

- **To change Purge Valve Times (Hewlett Packard 5890 Gas Chromatograph)**

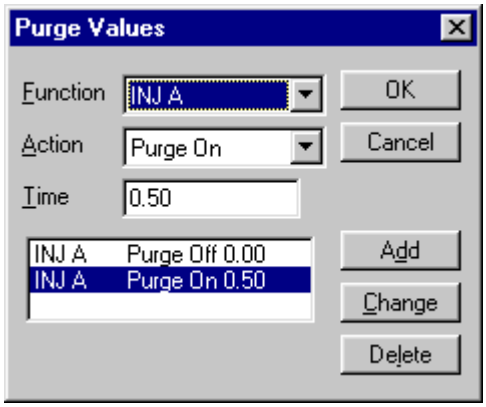


Figure 5.3 *HP5890 Purge Valve Editor*

Hewlett Packard 7673A Auto Injector

The HP 7673A auto injector can only be used with the HP 5890 gas chromatograph.

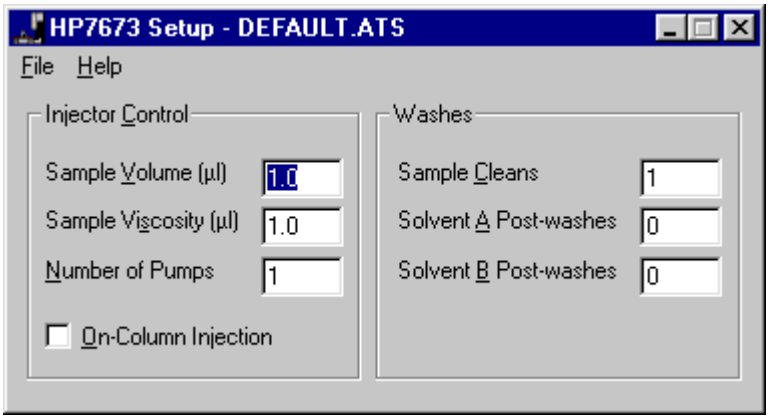


Figure 5.4 *HP7673A Auto Injector Editor*

Note: This dialog only applies if the Dice option is selected at setup, if the Dice option is not selected a "No parameters to set" message is displayed.

To Change Autosampler parameters (Hewlett Packard 7673A Auto Injector)

1. Choose **Set up Auto Injector** from the Acquisition Control Panel Instrument menu

   or

   Double click on the picture of the auto injector on the Acquisition Control Panel to display the HP7673A editor shown above.

2. Make any changes to the parameters.

3. Save the method using either **Save** or **Save As** from the File menu.

A full description of all the parameters in this editor is given in the *HP7673A Automatic Sampler Operating Manual*.

An autosampler will usually be used with the multiple sample acquisition page where further information such as bottle number will be entered. Starting an acquisition with an autosampler will be covered in the next section

Hewlett Packard HPLC Systems

The HP1050, HP1090 and HP1100 HPLC systems can be controlled from MassLynx. All three photo diode array (PDA) and UV detectors are supported.

The software can be used to control the pump during instrument tuning or acquisition and can be used to provide multi-sample acquisitions. Both isocratic and gradient modes of operation are supported.

The HP1050 is described in the examples below. Differences for the HP1090 and HP1100 are also described.

Hewlett Packard Sampler Configuration Page

Select the **HP1050 AutoSampler**, **HP1090 AutoSampler** or **HP1100 AutoSampler** from the **View** menu or press the  toolbar button.

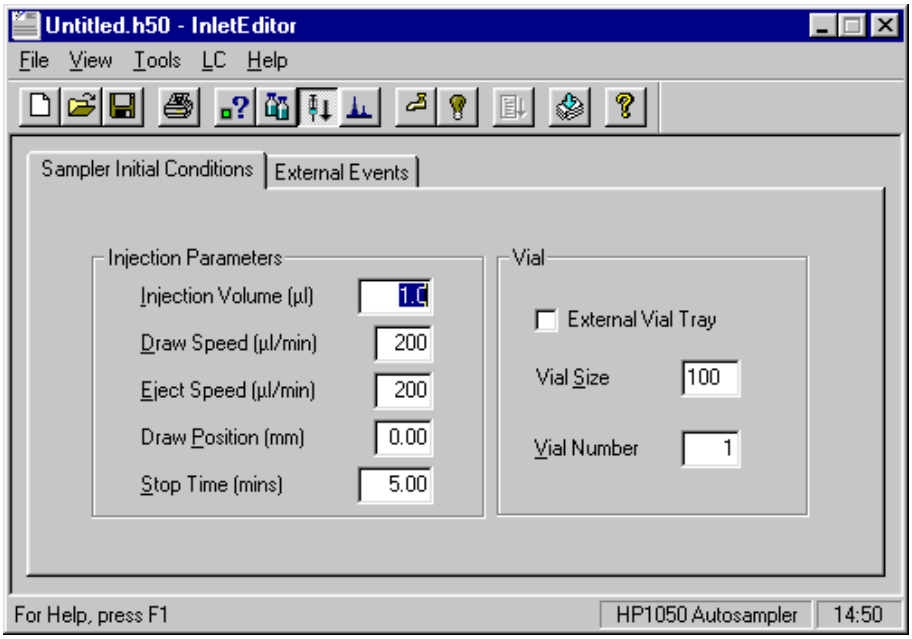


Figure 5.5 *HP1050 Sampler Initial Conditions Window*

Injection Volume This is the volume in microlitres to inject.

Note: If you are running from the Sample List the injection volume in the sample list entry overrides the setting defined here.

Draw Speed This determines the rate in microlitres per minute at which sample is extracted into the autosampler needle. This should be set according to the viscosity of your sample.

Eject Speed This is the speed in microlitres per minute at which sample is ejected from the needle on injection. Again set this according to the viscosity of the sample. Consult your HP documentation for further information. **Note:** This facility is only available with the HP1050 and HP1100 and will not be visible on an HP1090 system.

Draw Position This is an offset value in mm from position 0 and determines how far the needle is inserted into your sample. Consult your HP documentation for further information. Again this facility is only available with the HP1050 and HP1100 and will not be visible on an HP1090 system.

Stop Time This value is set in minutes to be the time that the autosampler method will run after injection. This does not apply to the HP1090 since this has an in-built autosampler.

External Vial Tray If an external vial tray is used check this box.

Vial number The vial to inject from.

Note: If a multisample acquisition is being run from the MassLynx Sample List, the Bottle # entry in the sample list overrides the value defined in the Vial Number box.

Syringe Size Set this to the size of syringe fitted on the HP1090 LC System. This parameter applies to the HP1090 only and will not be visible in a HP1050 or HP1100 system.

Thermostat On If the autosampler is fitted with a sample heater then this box will be enabled. Check it to use the sample heater. This parameter applies to the HP1100 only and will not be visible in a HP1050 or HP1090 system.

Sample Temperature Enter the temperature to heat the sample to. This parameter applies to the HP1100 only and will not be visible in a HP1050 or HP1090 system.

■ Hewlett Packard Sampler External Events Page

External events allow control of the external contacts found on the HP1050 and HP1090 LC systems. In addition HP1090 column switching can also be controlled. For the HP1100 a separate contact board must be installed in the pump in order to use this functionality.

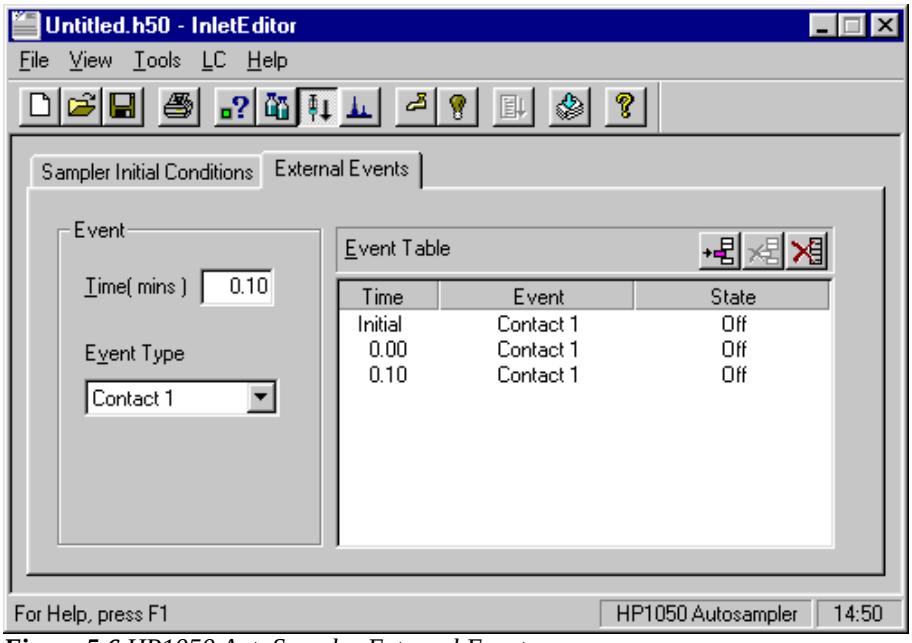


Figure 5.6 *HP1050 AutoSampler External Events page*

The contacts can be set to operate under timed control during a method run, as well as having their initial states set. The contacts will be in the initial state before a method run and will return to this state after a method has completed.

To add an event, enter a **Time**, select an **Event Type** from the drop down list box and press the toolbar button.

To delete a single event click with left mouse button on a time in the list and press the toolbar button.

To delete all entries press the toolbar button. This button is only available when there are entries in the timetable.

To change the **State** of a contact, double click on the time entry in the list to toggle between states.

Time The time in minutes at which the contact event should occur.

Event The contact event to be performed.

State The state determines whether the contact is to be opened or closed.

- **Hewlett Packard Pump Initial Conditions Page**

Select the **HP1050 Pump**, **HP1090 Pump** or **HP1100 Pump** from the **View** menu or press the toolbar button.

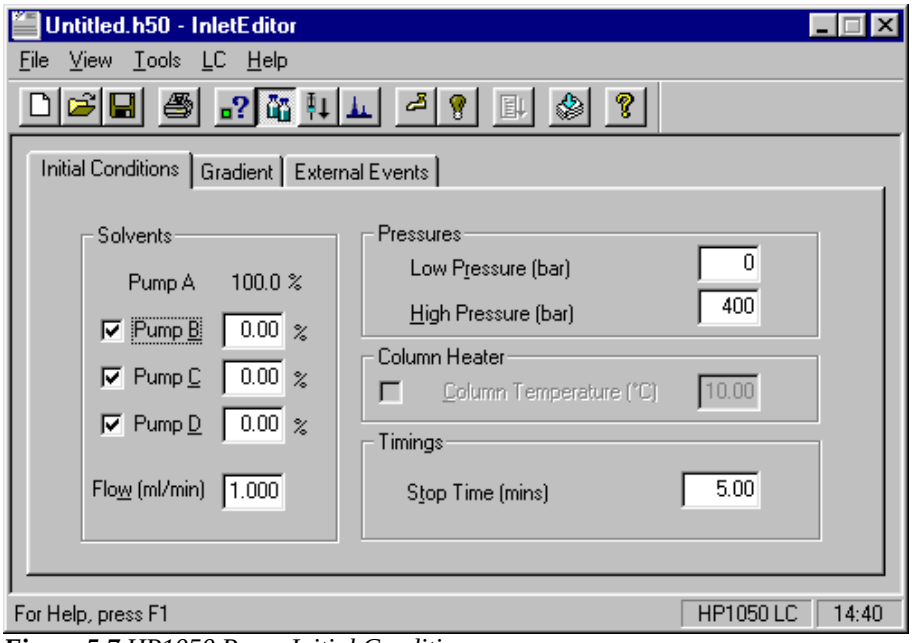


***Figure 5.7** HP1050 Pump Initial Conditions page*

Solvents Up to four solvents will be displayed depending upon the system configuration. The total value of all the solvent percentages added together must not exceed 100%.

Pump A This is the remainder percentage after the solvent percentages have been set for the other pumps.

Pump B, C, D These can either be enabled or disabled by checking the box next to the individual pumps. The values can be set to the required percentage of flow delivery.

Flow This is the total flow rate of the solvent channels according to how you have configured the instrument.

Pressures These set the upper and lower limits of the pressure within the solvent delivery system (SDS) if the pressure falls outside of this range the SDS switches off.

Column Heater If the instrument has an oven present then the column temperature can be set to a specified temperature in degrees centigrade. Check the Column Temperature box and enter a temperature. If the software has been configured to operate without a column oven then these boxes will be grayed out. **Note:** For the HP1100 a temperature should be entered in both the **Left** and **Right** boxes.

Stop Time This value is set to the time in minutes that the method will run from the point of injection.

- **Hewlett Packard Pump Gradient Timetable Page**

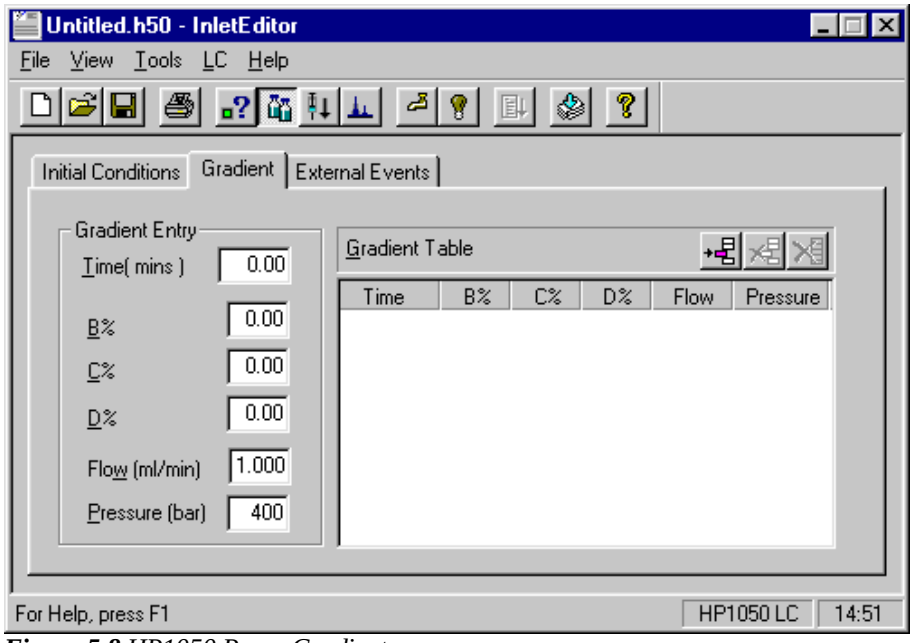


Figure 5.8 *HP1050 Pump Gradient page*

This page allows a gradient to be entered and edited. To operate in isocratic mode ensure the timetable is empty.

To add a gradient, type in a time and percentage in the relevant boxes and press the  toolbar button. **Note:** The first entry must have a time of 0.

To delete a single gradient, click with left mouse button on a time in the list and press the  toolbar button.

To delete all entries press the  toolbar button. This button is only available when there are entries in the timetable.

To modify a gradient, select the required entry in the timetable. The values will then be displayed in the edit boxes above the timetable, and can be altered as appropriate. Once changed press  to re-enter the values into the timetable. If, however, you modify the time value such that it does not correspond to any existing entry in the timetable pressing  will result in a new entry being created in the timetable.

The gradient parameters that you can set are as below. **Note:** The number of solvent percentages, which appear in the dialog, depends on which type of gradient was selected in the LC Configuration Window.

Time The time at which you wish the following parameters to be attained during a method run.

%B The percentage of solvent B you wish to attain at the given time.

%C The percentage of solvent C you wish to attain at the given time.

%D The percentage of solvent D you wish to attain at the given time.

Flow The required flow in ml/min that you wish to attain at the given time.

Pressure This is only available on the HP1050 and HP1100 and allows the limiting high pressure (in bars) to be reset at the given time.

■ Hewlett Packard Pump External Events Page

External events allow control of the external contacts found on the HP1050 and HP1090 LC systems. In addition HP1090 column switching can also be controlled. For the HP1100 you must have the separate contact board installed in your pump in order to use this functionality.

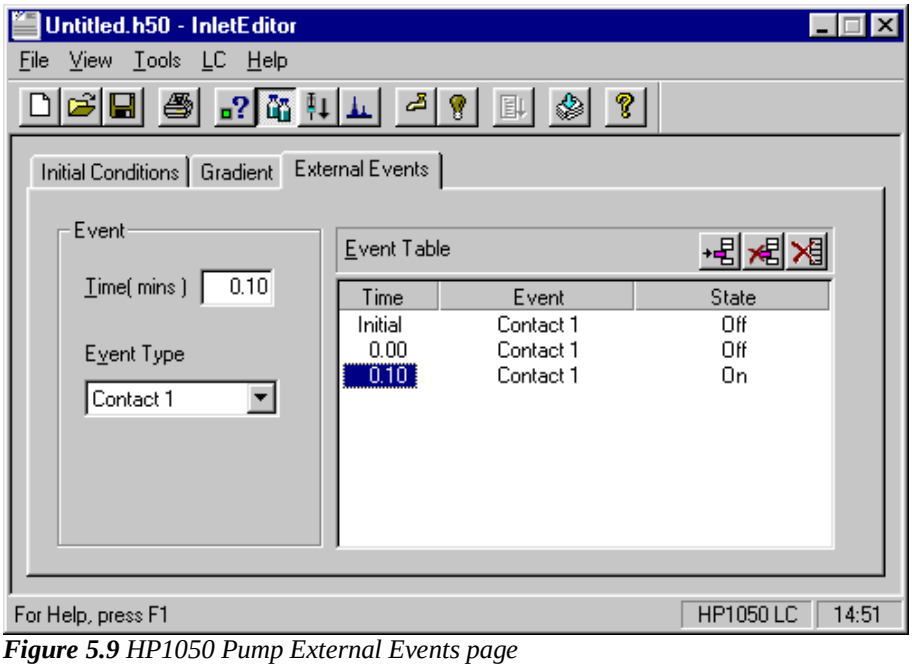


Figure 5.9 *HP1050 Pump External Events page*

The contacts can be set to operate under timed control during a method run, as well as having their initial states set. The contacts will be in the initial state before a method run and will return to this state after a method has completed.

To add an event, type in a **Time** and select an **Event Type** from the drop down list box and press the  toolbar button.

To delete a single event, click with left mouse button on a time in the list and press the  toolbar button.

To delete all entries press the  toolbar button. This button is only available when there are entries in the timetable.

To change the **State** of a contact, double click on the time entry in the list to toggle between states.

Time The time in minutes at which you would like the contact event to occur.

Event Type This determines the contact event to be displayed in the list of events. Once displayed, the events can be added, deleted or changed as described above.

State The state determines whether the contact is to be opened or closed.

To Set-up the Diode Array Detector (Hewlett Packard)

Select the **HP1050 PDA Detector** from the **View** menu or press the  toolbar button.

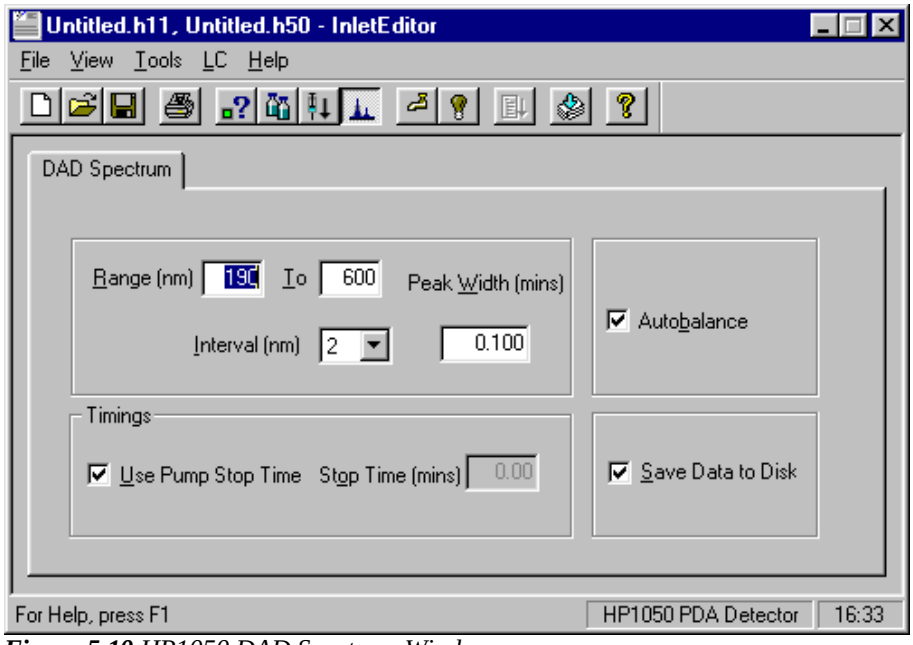


Figure 5.10 *HP1050 DAD Spectrum Window*

Range Enter the minimum (**Range**) and maximum (**To**) wavelengths in nanometers over which diode array spectral data will be acquired.

Peak Width Determines the rate at which the data is acquired. There are approximately eight spectra per peak so a peak width of 0.1 minutes means eight spectra will be acquired every 6 seconds.

Interval This determines the number of spectral data points acquired. For example an interval of 4 nanometers means data points will be acquired at the lower wavelength, the lower wavelength plus 4nm and so on.

Autobalance Check this box to zero the base line of the diode array detector before each analysis.

Use Pump Stop Time Check this box use the **Stop Time** defined on the Pump Initial Conditions page (see page 130).

Stop Time This option is not enabled if the **Use Pump Stop Time** box is checked. It determines the time in minutes the diode array method will run. Data will be acquired for this amount of time.

Save Data to Disk Check this box to store the diode array data to disk. If you do not wish to save the diode array data to disk you should uncheck this box.

- **HP1100 DAD**

The HP1100 DAD dialog has **Pre Autobalance** and **Post Autobalance** in place of **Autobalance**. Check the relevant box to zero the baseline of the diode array detector before or after each analysis.

- **Hewlett Packard 1050 UV Detector**

Select **HP1050 UV Detector** from the **View** menu or press the  toolbar button.

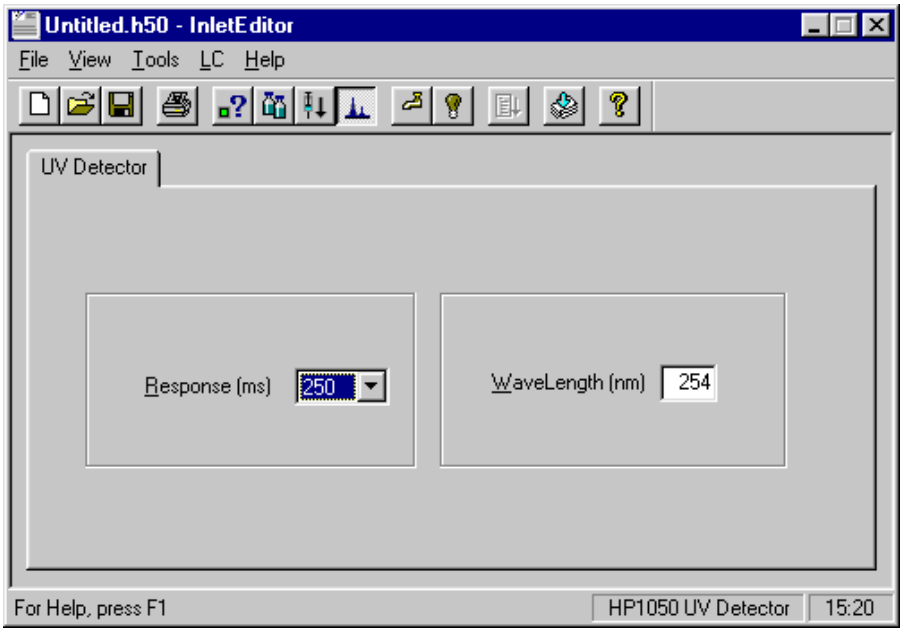


Figure 5.11 *HP1050 UV Detector Window*

Response Select 250, 1000 or 4000 msec from the drop down list box.

Wavelength Enter the wavelength in nanometers to be monitored.

Hewlett Packard 1090 UV Detector

Select **HP1090 UV Detector** from the **View** menu or press the  toolbar button.

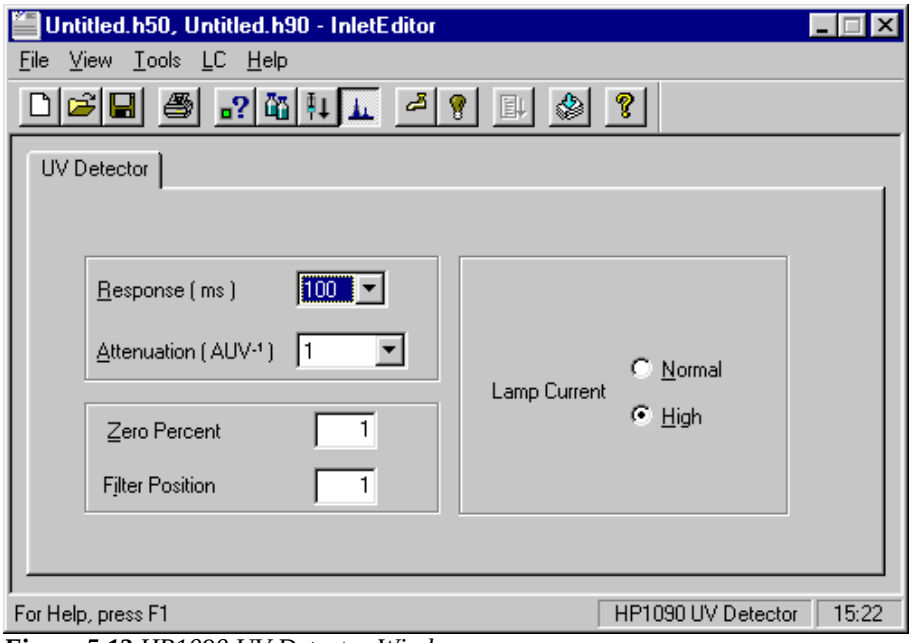


Figure 5.12 *HP1090 UV Detector Window*

Response Select one of the values from the drop down list.

Attenuation Select one of the values from the drop down list.

Zero Percent Increase the value to increase the baseline.

Filter Position Set this to the number of the filter required.

Lamp Current Set to Normal or High.

Hewlett Packard 1100 UV Detector

Select **HP1100 UV Detector** from the **View** menu or press the  toolbar button.

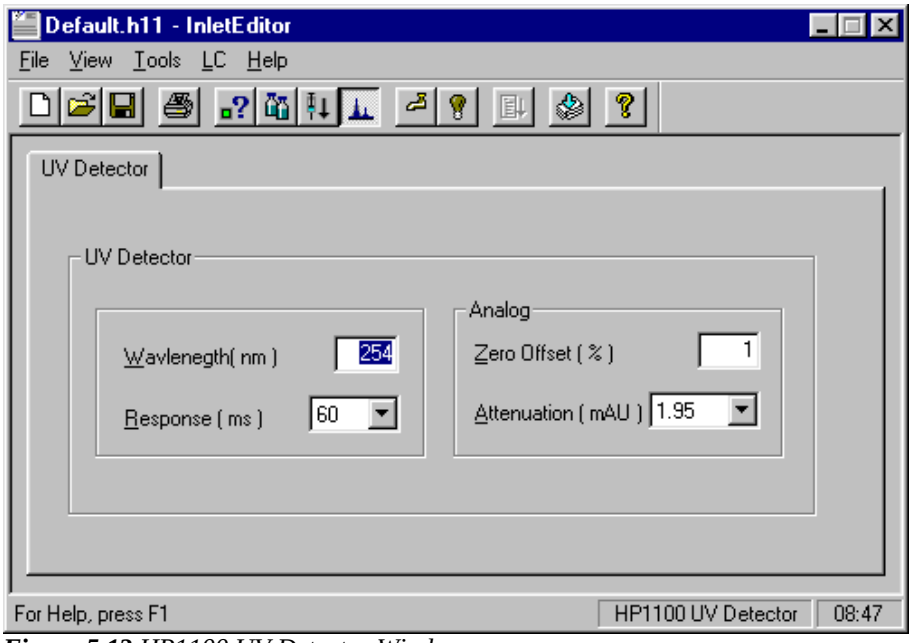


Figure 5.13 *HP1100 UV Detector Window*

Wavelength Set to the wavelength in nanometers to be monitored.

Response Select one of the values from the drop down list.

Zero Offset Increase the value to increase the baseline.

Attenuation Select one of the values from the drop down list.

The HP6890 System Status Page

The System Status page displays information about the state of the machine being controlled. This page can be accessed from the Inlet Editor by selecting **Status** from the **View** menu or by pressing the  toolbar button.

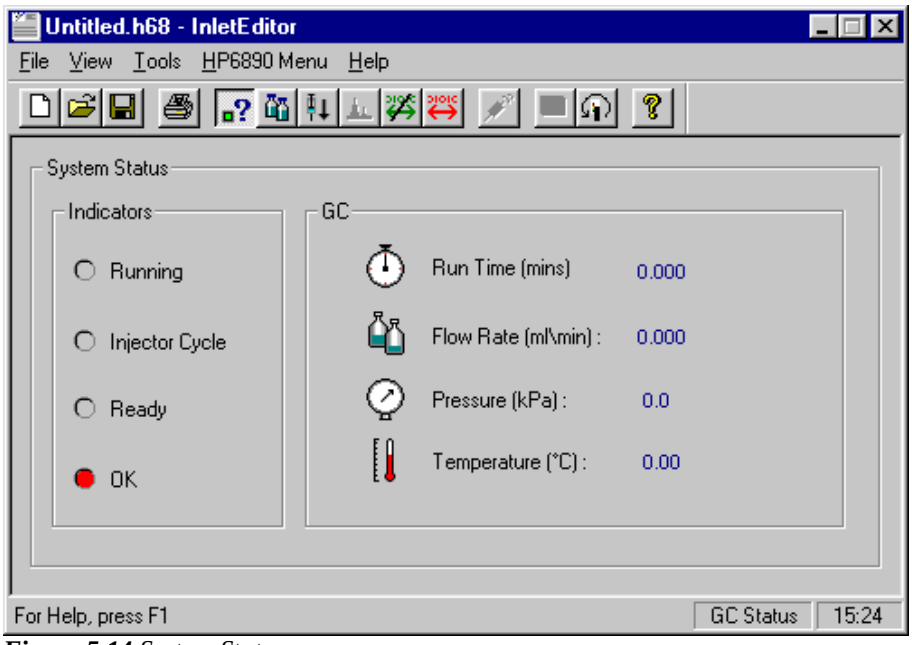


Figure 5.14 *System Status page*

Indicators The Running and Injector Cycle indicators at the left of the screen give information on the current status of the GC system. The OK and Ready Indicators become illuminated in red if the GC System has an error. Click on the red indicators to display more information on the cause of the error.

Run Time This displays how long the method has been running.

Flow Rate This is the current flow rate as returned by the instrument. The current value will be the setpoint when using a flow based mode or the actual flow if in a pressure based mode.

Pressure This displays the current pressure in the instrument. The current value will be the setpoint when using a pressure based mode or the actual pressure if in a flow based mode.

Temperature This displays the current oven temperature of the GC.

HP6890 Sampler Configuration Page

Select the **HP6890 AutoSampler** from the **View** menu or press the  toolbar button.

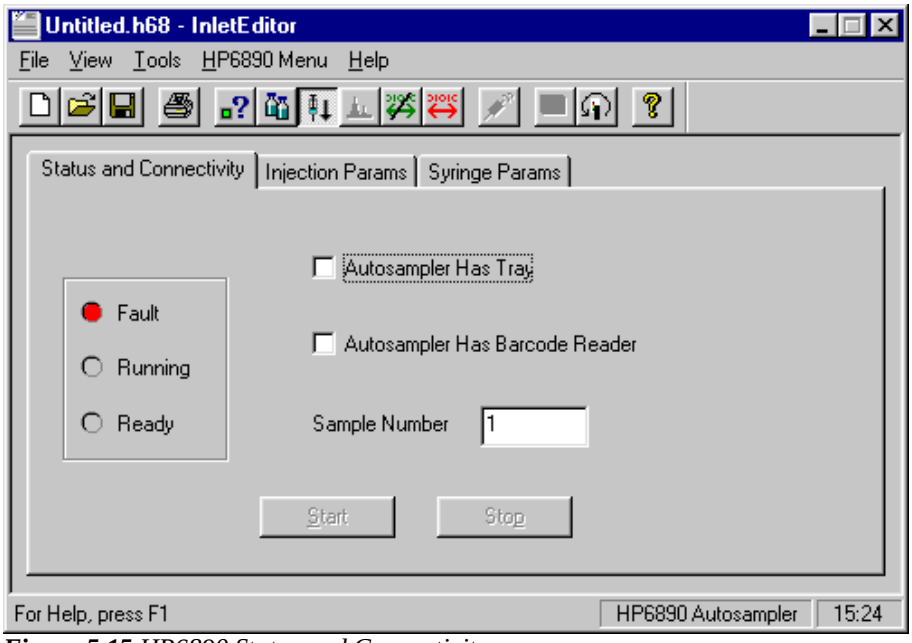


Figure 5.15 *HP6890 Status and Connectivity page*

Fault A red light indicates that the Autosampler has developed a fault.

Running A green light indicates that the Autosampler is active. The Autosampler is active if it is moving a vial, rinsing or injecting.

Ready A green light indicates that the Autosampler is ready to start processing another vial.

Autosampler Has Tray Check this box if the Autosampler has a tray.

Autosampler Has Barcode Reader Check this box if the Autosampler has a barcode reader.

Sample Number Enter the vial number that the injection will be taken from, when the start button is pressed.

Start Press this button to start an autosampler (and hence GC) run with the currently stored method.

Stop Press this button to stop the Autosampler. It will not stop a GC run.

- **HP6890 Injection Params Page**

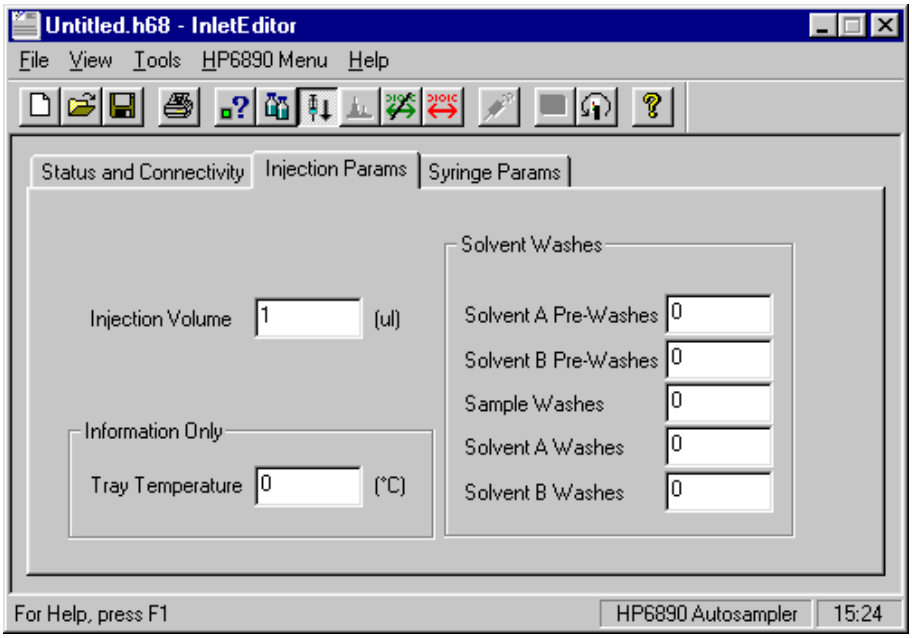


Figure 5.16 *HP6890 Injection Parameters page*

Injection Volume Enter the injection volume to be used for a run started using the Start button on the Status and Connectivity page. **Note:** If the acquisition is started from the Sample List then this value will be overridden by the sample list injection volume.

Tray Temperature This is used for record purposes only and is the tray temperature at which this method is normally used.

Solvent Washes These allow a rinse strategy for each sample to be set up. Enter the number of washes of each type in the required boxes.

- **HP6890 Syringe Params Page**

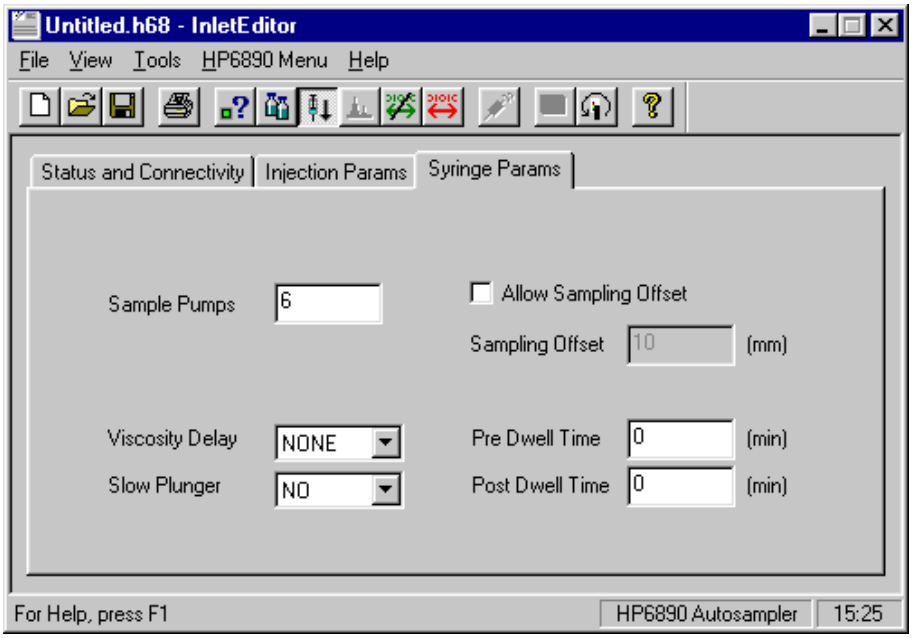


Figure 5.17 *HP6890 Syringe Parameters page*

Sample Pumps Enter the number of times the syringe will draw in liquid in order to fill it.

Viscosity Delay Select the length of time that the needle will stay in the vial to ensure that all the sample has been drawn into the syringe, from the drop down list box.

Slow Plunger For viscous liquids select **YES** from the drop down list box otherwise select **NO**.

Allow Sampling Offset Check this box to enable the Sampling Offset.

Sampling Offset Enter the distance from the bottom of the vial (in millimeters) that the injection will be taken from. This is to allow samples to be taken from different parts of a multi-phased sample. **Note:** This box will bot be enabled unless the **Allow Sampling Offset** box is checked.

Pre Dwell Time and **Post Dwell Time** If, for example the sample needs heating before injection, the syringe needle can be held in the GC inlet for **Pre Dwell Time** and/or **Post Dwell Time**. Enter the length of time in the relevant box.

- **To Set-up the Pump (HP6890)**

Select the **HP6890 Pump** from the **View** menu or press the  toolbar button.

- **HP6890 Status Page**

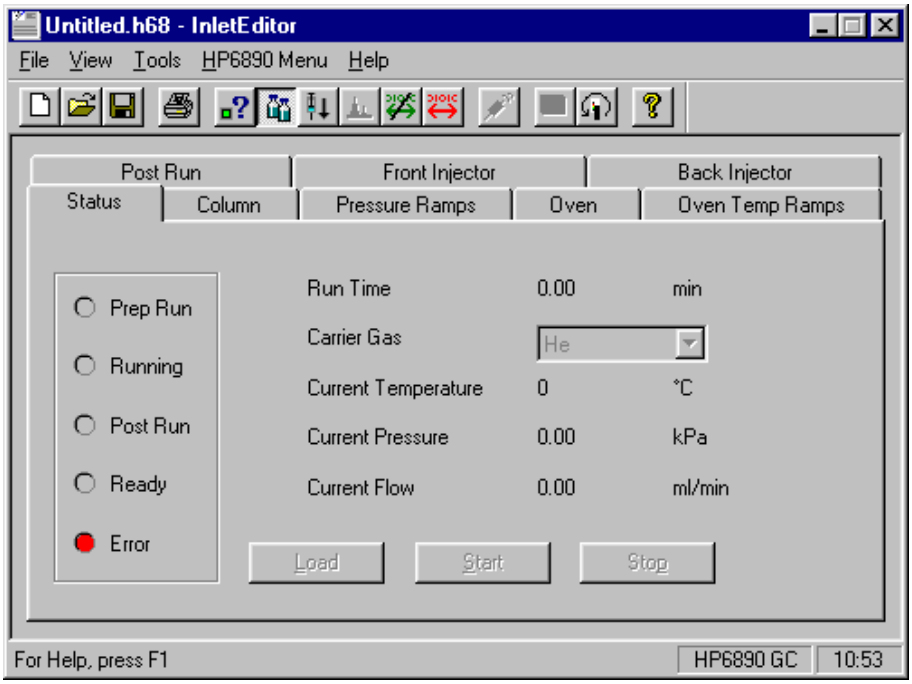


Figure 5.18 *HP6890 GC Status page*

Prep Run This will be yellow when the GC is in the Prep Run state. This occurs when the GC is trying to equilibrate before an automatic injection start.

Running This will be yellow when the GC is in the Running state. This occurs when the GC has started its temperature and/or pressure profiles for a run.

Post Run This will be yellow when the GC is in the Post Run state.

Ready This will be green when the GC is equilibrated and ready to start a run.

Error This will be red when the GC is in an Error state or there is a communication problem between the GC and the Host (local PC).

The **Run Time**, **Current temperature**, **Current Pressure** and **Current Flow** are described in the System Status Page on page 137. **Carrier Gas** is described below.

- **HP6890 Column Page**

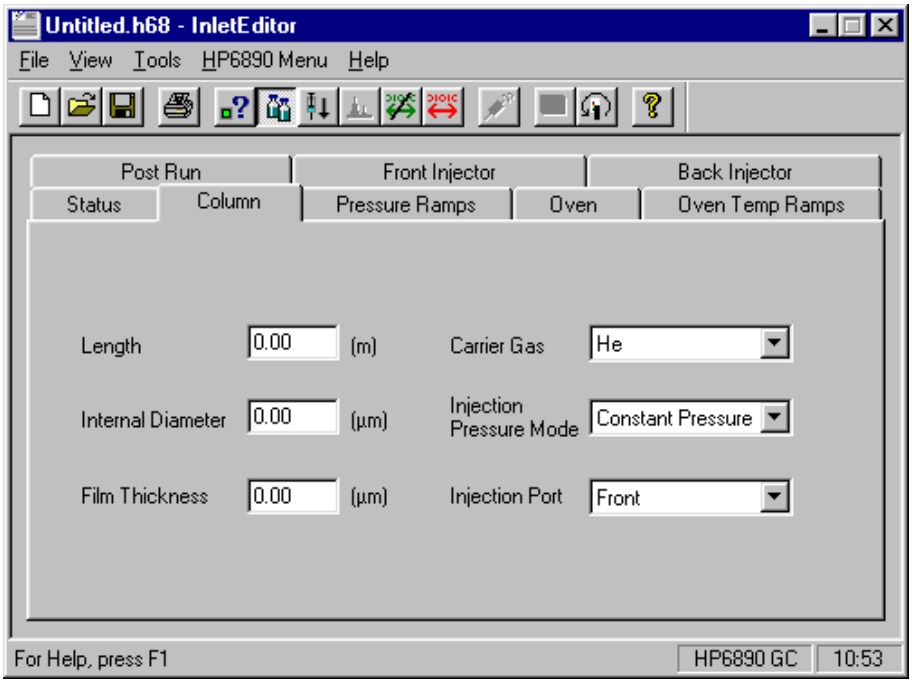


Figure 5.19 *HP6890 Column page*

Length Enter the column length in meters.

Internal Diameter Enter the internal diameter of the column in micrometers.

Film Thickness Enter the thickness of the column coating in micrometers.

Carrier Gas Select a carrier gas from the drop down list box.

Injection Pressure Mode Select Constant Pressure, Ramped Pressure, Constant Flow or Ramped Flow from the drop down list box.

Injection Port Select Front or Back from the drop down list box.

HP6890 Pressure Ramps Page

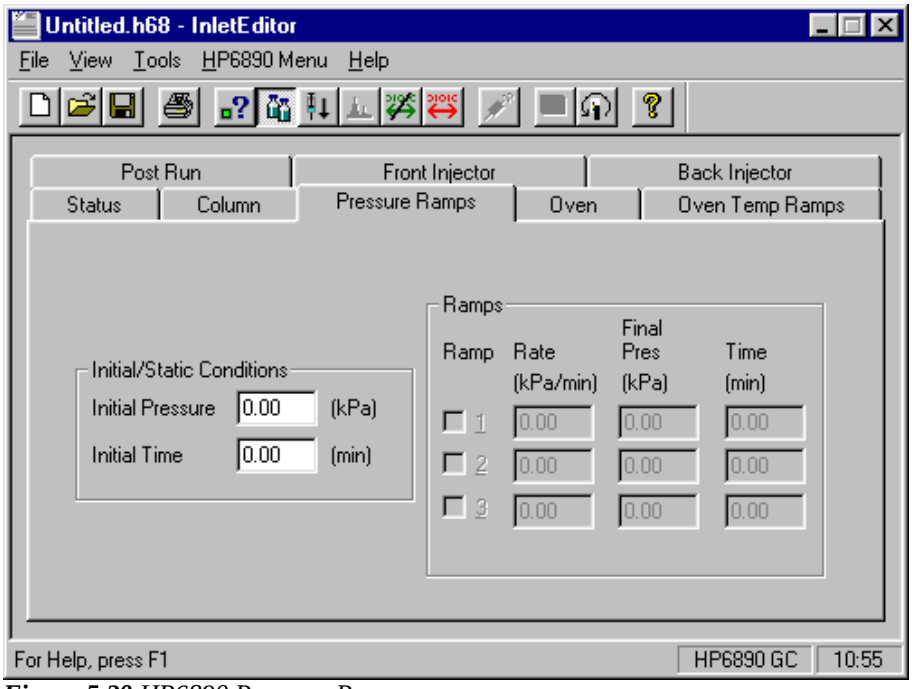


Figure 5.20 *HP6890 Pressure Ramps page*

This appearance of this page will vary depending on the Injection Pressure Mode selected on the Column page. If Constant Pressure was selected only Initial Pressure and Initial Time are enabled. If Ramped Pressure was selected then the Ramps are enabled as well. If Constant Flow or Ramped Flow was selected, the parameters will be as for the corresponding Pressure page but Pressure will be replaced by Flow.

Initial Pressure/Flow Enter the pressure/flow required for the Initial state.

Initial Time Enter the length of time to remain at the initial pressure/flow

Ramps To enable a Ramp check the relevant Ramp box or enter a non-zero value in the Rate box.

Rate Enter rate of pressure/flow change for current ramp.

Temp Enter final pressure/flow for current ramp.

Time Enter the length of time to remain at the final pressure/flow of current ramp, before proceeding to the next ramp.

HP6890 Oven Page

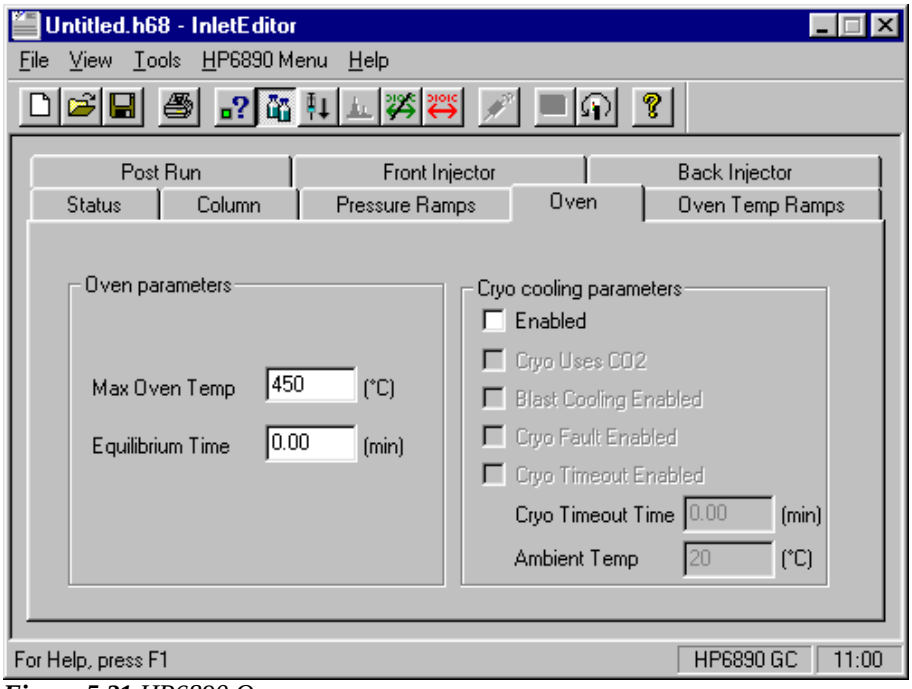


Figure 5.21 *HP6890 Oven page*

Max Oven Temp Enter the maximum oven temperature. Temperatures entered in the ramps on the other pages will not be accepted if they exceed this parameter.

Equilibrium Time Enter the time to wait at the Initial Temperature (defined on subsequent pages) before the ready signal is displayed.

Cryo cooling parameters To enable these parameters check the **Enabled** box.

Cryo Uses CO2 Check this box if the cryo system uses CO_2 instead of N_2.

Blast Cooling Enabled Check this box if the cryo system is to be used above ambient temperatures to speed up cooling of the oven.

For a detailed description of **Cryo Fault** & **Timeout** consult your HP6890 manual or site engineer.

Ambient Temp Enter the temperature regarded as normal ambient around the GC.

HP6890 Oven Temp Ramps Page

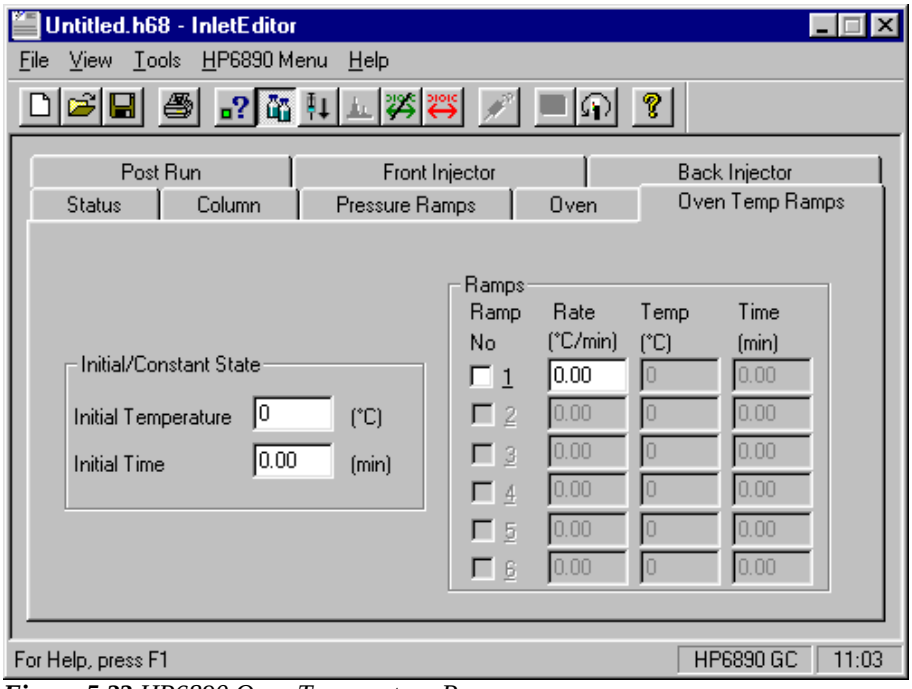


Figure 5.22 *HP6890 Oven Temperature Ramps page*

Initial Temperature Enter the temperature required for the Initial State.

Initial Time Enter the length of time to remain at the initial temperature.

Ramps To enable a Ramp check the relevant **Ramp No** box or enter a non-zero value in the Rate box.

Rate Enter rate of temperature change for current ramp.

Temp Enter final temperature for current ramp.

Time Enter the length of time to remain at the final temperature of the current ramp, before proceeding to the next ramp.

HP6890 Post Run Page

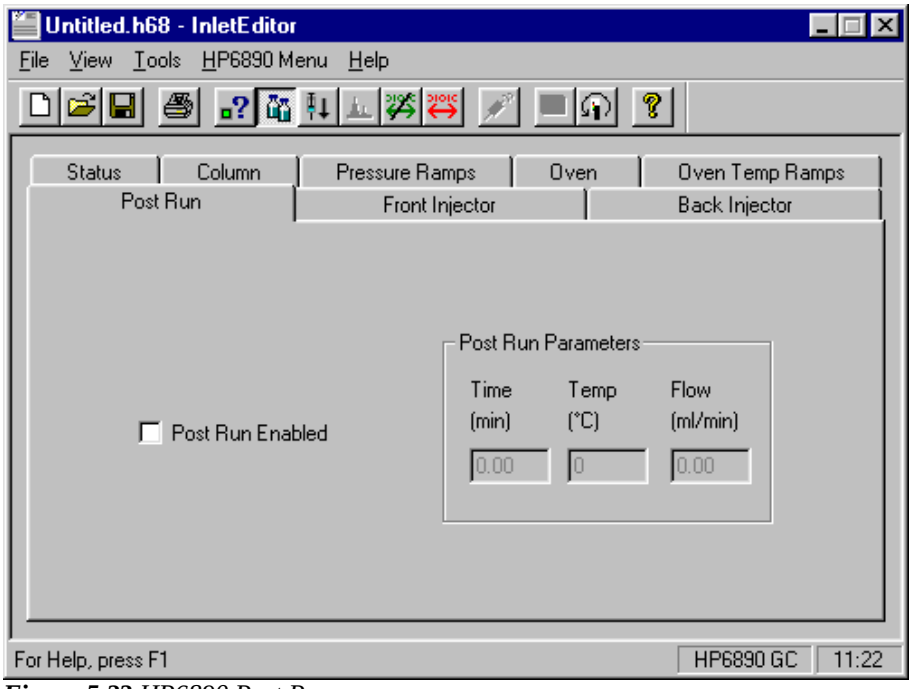


Figure 5.23 *HP6890 Post Run page*

This appearance of this page will vary depending on the Injection Pressure Mode selected on the Column page. If Constant Pressure or Ramped Pressure was selected then a Post Run Pressure is required. If Constant Flow or Ramped Flow was selected then a Post Run Flow is required.

Post Run Enabled Check this box if a Post Run is required.

Time Enter the length of time for the post run phase.

Temp Enter the temperature for the post run phase.

Pressure/Flow Enter the head pressure/flow for the post run phase.

- **HP6890 Front and Back Injector Pages**

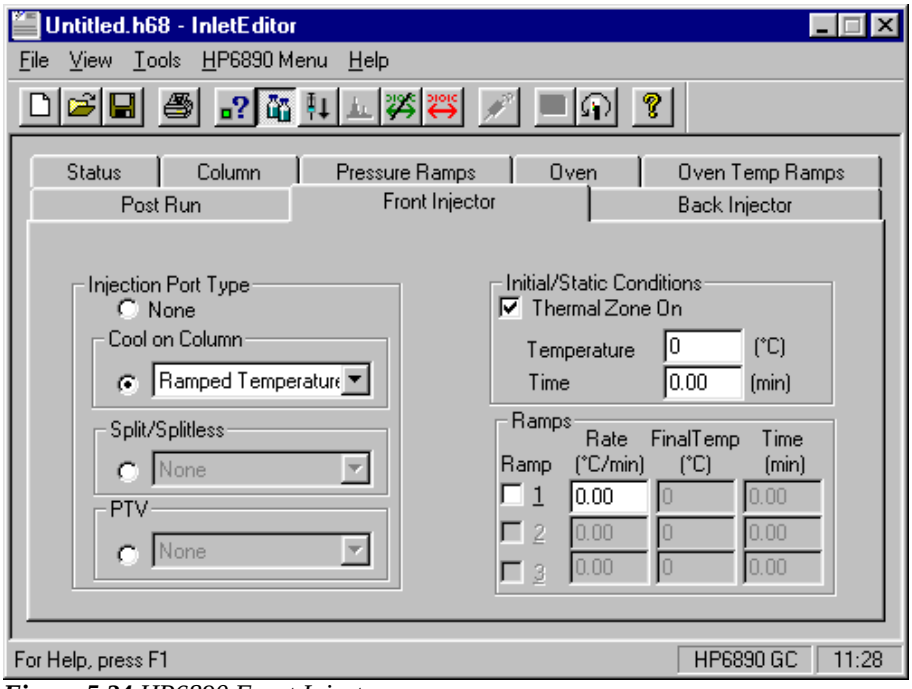


Figure 5.24 *HP6890 Front Injector page*

Injection Port Type If **None** is selected there are no parameters to enter.

Cool on Column

If **Track Oven** is selected there are no parameters to enter.

If **Ramped Temperature** is selected **Figure 5.24** is displayed.

Thermal Zone On Check this box to enable the **Temperature**, **Time** and **Ramps** fields.

The Initial/Static conditions and Ramps details are used to provide a temperature profile for the inlet independent to the temperature profile of the oven, but the method of use is the same.

Initial Temperature Enter the temperature required for the Initial State.

Initial Time Enter the length of time to remain at the initial temperature.

Ramps To enable a Ramp check the relevant Ramp box or enter a non-zero value in the Rate box.

Rate Enter rate of temperature change for current ramp.

Final Temp Enter final temperature for current ramp.

Time Enter the length of time to remain at the final temperature of the current ramp, before proceeding to the next ramp.

Split/Splitless

If **None** is selected there are no parameters to enter.

If **Split** is selected **Figure 5.25** is displayed.

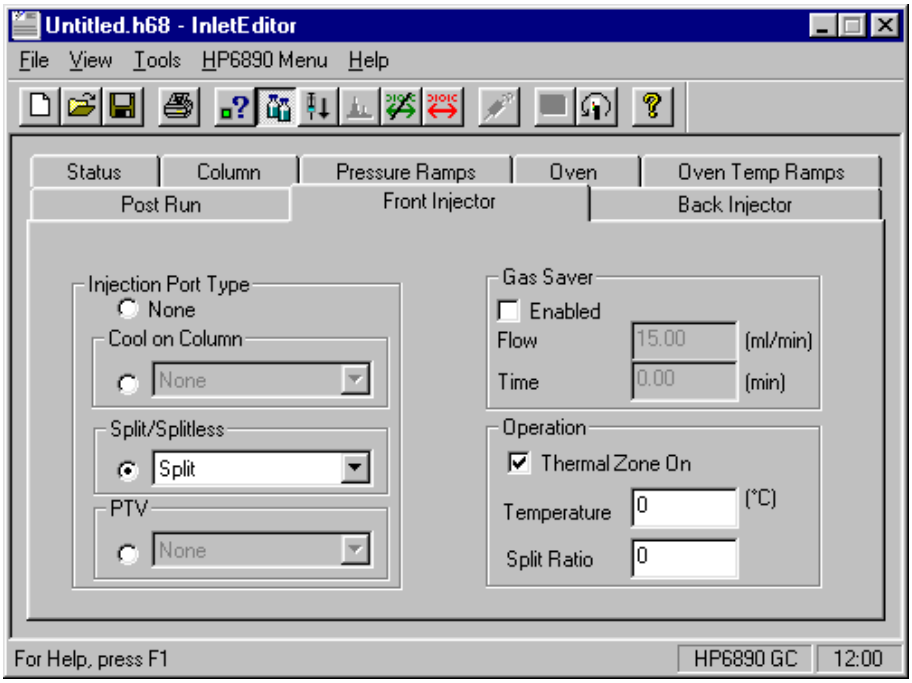


Figure 5.25 *HP6890 Front Injector page - Split*

Gas Saver Enabled Check this box to save gas after an injection.

Note: Auto prep run must be manually set to ON if this box is checked. See the HP6890 manual for details.

Flow Enter the reduced flow rate.

Time Enter the length of time to deliver the reduced flow rate for.

Thermal Zone On Check this box to enable the **Temperature** and **Split Ratio** fields.

Temperature Enter the temperature at which to hold the inlet during the run.

Split Ratio Enter the split ratio for the inlet flow.

If **Splitless** is selected **Figure 5.26** is displayed.

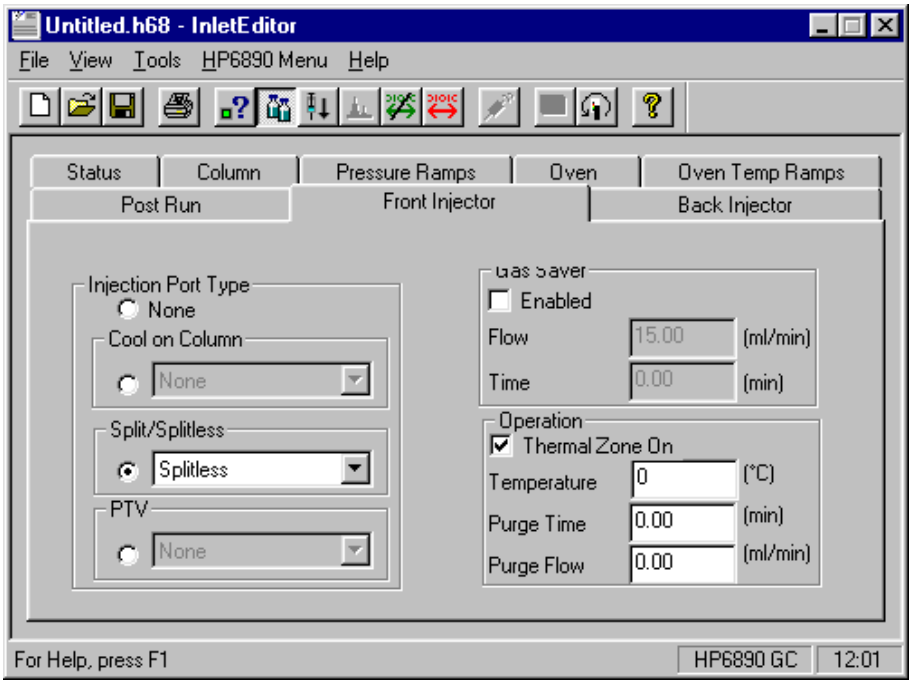


***Figure 5.26** HP6890 Front Injector page - Splitless*

Gas Saver Enabled Check this box to save gas after an injection.

Note: Auto prep run must be manually set to ON if this box is checked. See the HP6890 manual for details.

Flow Enter the reduced flow rate.

Time Enter the length of time to deliver the reduced flow rate for.

Thermal Zone On Check this box to enable the **Temperature**, **Purge Time** and **Purge Flow** fields.

Temperature Enter the temperature at which to hold the inlet during the run.

Purge Time Enter the time at which to open the purge valve.

Purge Flow Enter the flow rate to use at the Purge Time.

PTV

If **None** is selected there are no parameters to enter.

If any other option is selected **Figure 5.27** is displayed.

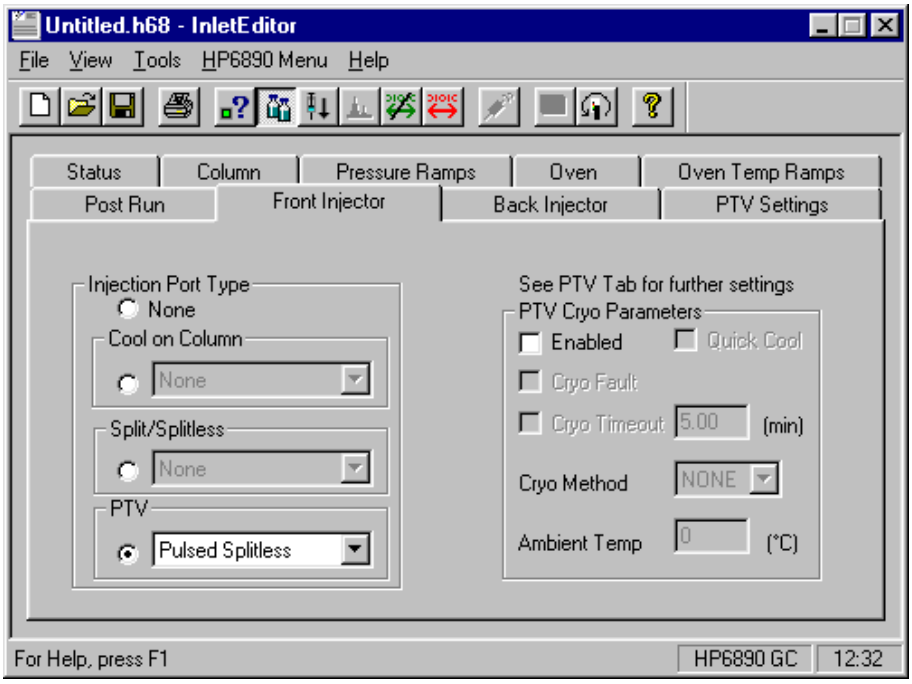


***Figure 5.27** HP6890 Front Injector page*

PTV Cryo Parameters Enabled Check this box enable the other options on this dialog.

Quick Cool Check this box to Enter the reduced flow rate.

Time Enter the length of time to deliver the reduced flow rate for.

Thermal Zone On Check this box to enable the **Temperature** and **Split Ratio** fields.

Temperature Enter the temperature at which to hold the inlet during the run.

Split Ratio Enter the split ratio for the inlet flow.

Max Oven Temp Enter the maximum oven temperature.

Equilibrium Time Enter the time required to reach equilibrium at the new temperature.

Cryo cooling parameters To enable these parameters check the **Enabled** box.

Cryo Uses CO2 Check this box if the cryo system uses CO_2 instead of N_2.

Blast Cooling Enabled Check this box if the cryo system is to be used above ambient temperatures to speed up cooling of the oven.

For a detailed description of **Cryo Fault** & **Timeout** consult your HP6890 manual or site engineer.

Ambient Temp Enter the temperature regarded as normal ambient around the GC.

Flow Enter the reduced flow rate.

Time Enter the length of time to deliver the reduced flow rate for.

Thermal Zone On Check this box to enable the **Temperature**, **Purge Time** and **Purge Flow** fields.

Temperature Enter the temperature at which to hold the inlet during the run.

Purge Time Enter the time at which to open the purge valve.

Purge Flow Enter the flow rate to use at the Purge Time.

The Back Injector parameters are edited in the same way as those for the Front injector.

PTV Settings Page

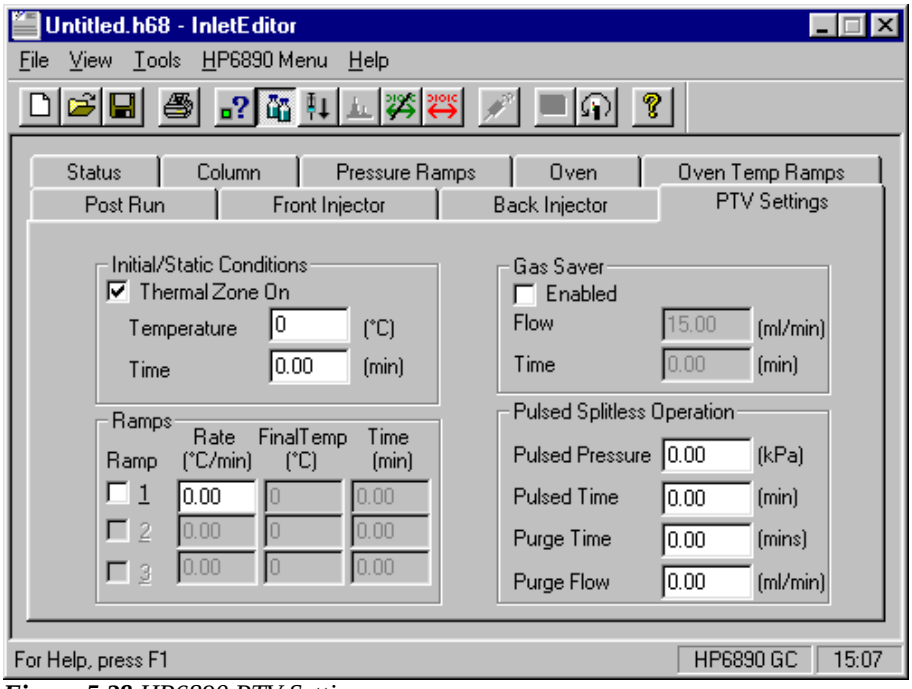


Figure 5.28 *HP6890 PTV Settings page*

Thermal Zone On Check this box to enable the **Temperature**, **Time**, **Ramps** and **Pulsed Splitless Operation** fields.

The Initial/Static conditions and Ramps details are used to provide a temperature profile for the inlet independent to the temperature profile of the oven, but the method of use is the same.

Initial Temperature Enter the temperature required for the Initial State.

Initial Time Enter the length of time to remain at the initial temperature.

Ramps To enable a Ramp check the relevant Ramp box or enter a non-zero value in the Rate box.

Rate Enter rate of temperature change for current ramp.

Final Temp Enter final temperature for current ramp.

Time Enter the length of time to remain at the final temperature of the current ramp, before proceeding to the next ramp.

Gas Saver Enabled Check this box to save gas after an injection.

Note: Auto prep run must be manually set to ON if this box is checked. See the HP6890 manual for details.

Flow Enter the reduced flow rate.

Time Enter the length of time to deliver the reduced flow rate for.

Pulsed Pressure Enter the temperature at which to hold the inlet during the run.

Pulsed Time Enter the time at which to open the purge valve.

Purge Time Enter the time at which to open the purge valve.

Purge Flow Enter the flow rate to use at the Purge Time.

- **HP6890 Communication Parameters**

Select **View Comms Settings** from the **HP6890 Menu** or press the  toolbar button to view the current communications settings.

Communication settings should only be changed by an engineer, the **Edit Comms Settings** and the  toolbar button allow this to be done.

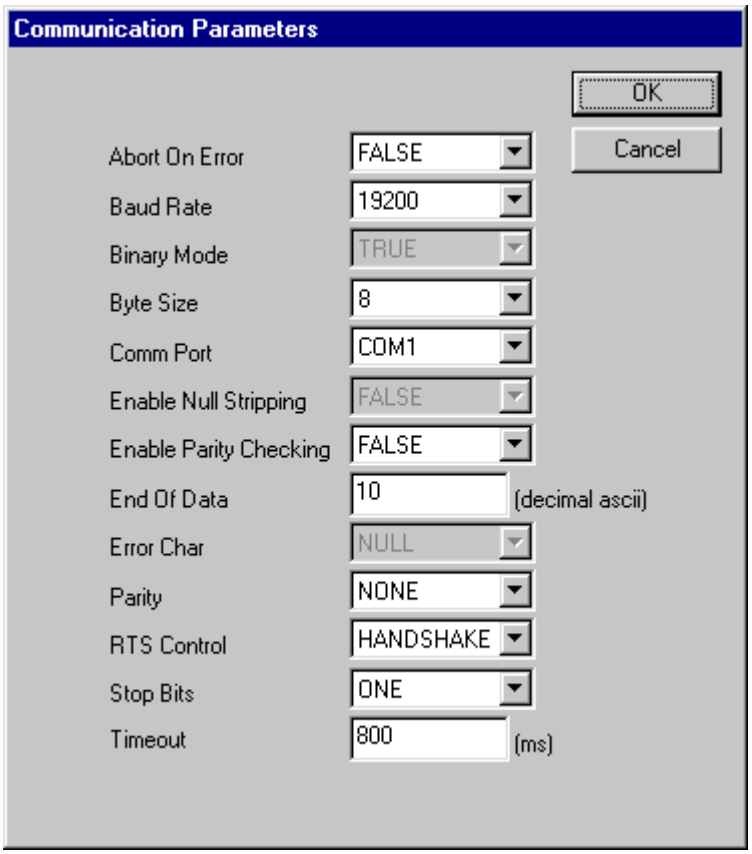


Figure 5.29 *HP6890 Communications Parameters dialog*

The HP6890 Toolbar

The HP6890 toolbar has five extra buttons on it, which are:

Click	To
	View current communications settings.
	Edit current communications settings.
	Start and stop method.
	Turn GC on and off.
	Reset Autosampler

Notes

Notes

Jasco Systems

Chapter 6

Jasco 900 and Jasco 1500 Autosamplers

The Inlet Editor for the Jasco 900 and Jasco 1500 autosamplers is the same. The Jasco 900 is used in the following examples.

- **Jasco Sampler Initial Conditions Page**

This page is used to set parameters specific to the Sampler, to access it select **Jasco900 AutoSampler** from the **View** menu or press the  toolbar button.

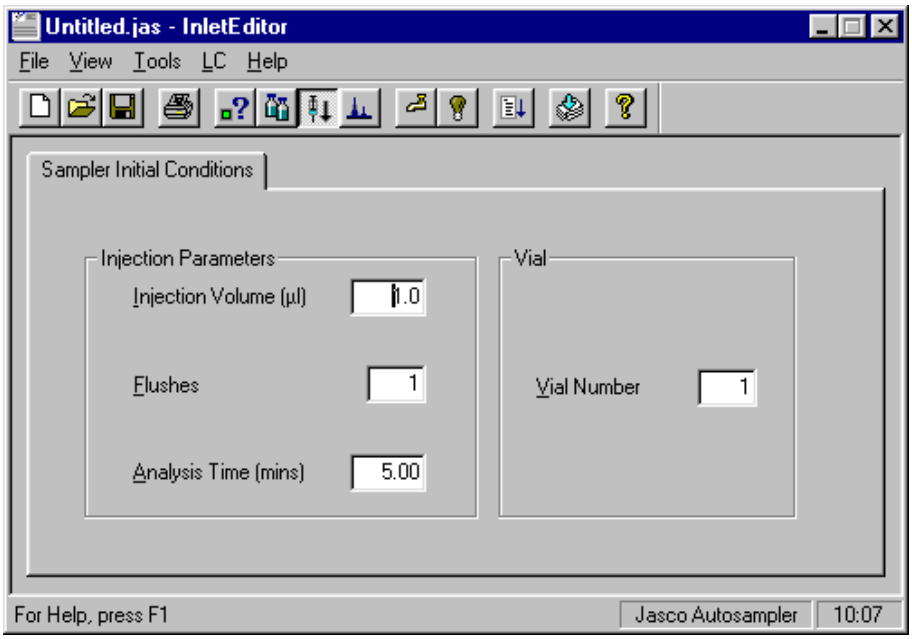


Figure 6.1 *Sampler Initial Conditions page*

Injection Volume Enter the volume in microlitres to inject.

Note: If a multisample acquisition is being run from the MassLynx Sample List, the injection volume defined in the sample list overrides the value defined here.

Flushes Enter the number of times the needle should be flushed between injections.

Analysis Time Enter the length of time the run will last for.

Vial number Enter the number of the vial to inject from.

Note: If a multisample acquisition is being run from the MassLynx Sample List, the Bottle # entry in the sample list overrides the value given in the Vial Number entry above.

Jasco 900 and Jasco 1500 Pumps

The Inlet Editor for the Jasco 900 and Jasco 1500 pumps is the same. The Jasco 900 is used in the following examples.

The Jasco Pump pages can be accessed by selecting **Jasco900 Pump** from the **View** menu on the Inlet Editor or by pressing the  toolbar button.

- **Jasco Initial Conditions Page**

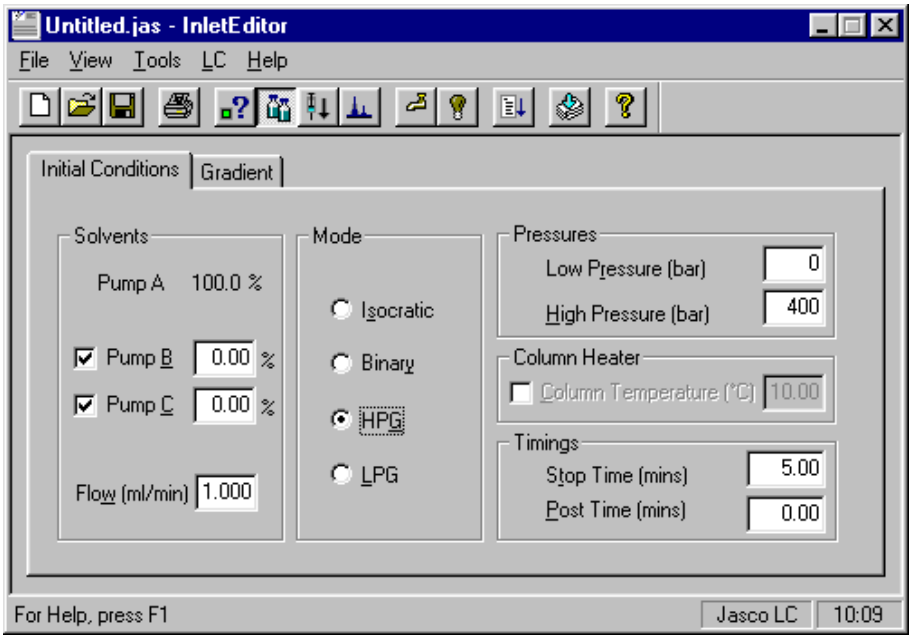


Figure 6.2 *Initial Conditions page*

Solvents Up to three solvents will be displayed depending upon the system configuration. The total value of all the solvent percentages added together must not exceed 100%.

Pump A This is the remainder percentage after the solvent percentages have been set for the other pumps.

Pump B and **C** Check the box for the pump required and enter the percentage of flow to deliver from this pump. To disable the pump, uncheck the box.

Flow This is the total flow rate of the solvent channels.

Mode Select **Isocratic** (One pump), **Binary** (Two pumps), **HPG** (High Pressure Gradient) or **LPG** (Low Pressure Gradient).

Pressures Enter the upper and lower limits of the pressure within the solvent delivery system (SDS), if the pressure falls outside of this range the SDS switches off.

Column Heater If the instrument has an oven present then the column temperature can be set to a specified temperature in degrees centigrade. Check the Column Temperature box and enter a temperature. If the software has been configured to operate without a column oven then these boxes will be greyed out.

Stop Time Enter the time in minutes that the method will run from the point of injection. If a Jasco Autosampler has also been selected, Analysis Time on the autosampler page overrides this value.

Post Time Enter the time in minutes that the instrument will run in its initial conditions after a method has completed. No further injections can be carried out whilst the system is in postrun thus allowing re-equilibration of the column.

Jasco Gradient Page

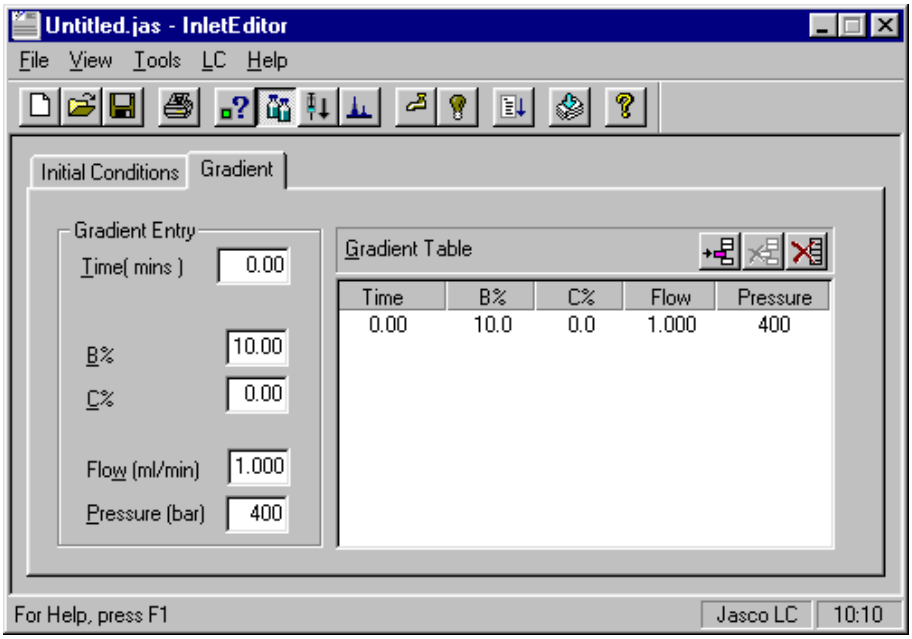
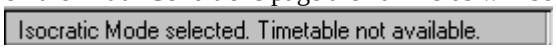


Figure 6.3 *Gradient Timetable page*

This page allows a gradient to be entered and edited. If isocratic mode was selected on the Initial Conditions page then all fields will be greyed out and



is displayed.

To add a gradient, enter a time and percentage in the relevant boxes and press the  toolbar button. **Note:** The first entry must have a time of 0.

To delete a single gradient, click with left mouse button on a time in the list and press the  toolbar button.

To delete all entries press the  toolbar button. This button is only available when there are entries in the timetable.

To modify a gradient select the required entry in the timetable. The values will then be displayed in the edit boxes to the right of the timetable and can be altered as appropriate. Once changed press  to re-enter the values into the timetable.
Note: If the time is changed and the new time does not correspond with an existing entry in the table, then a new entry will be added. If the new time correspond to an existing entry then the entry at that time will be overwritten.

Jasco 900 and Jasco 1500 UV Detectors

The Inlet Editor for the Jasco 900 and Jasco 1500 UV detectors is the same. The Jasco 900 is used in the following examples.

This page is used to set parameters specific to the UV detector, to access it select **Jasco900 UV Detector** from the **View** menu or press the  toolbar button.

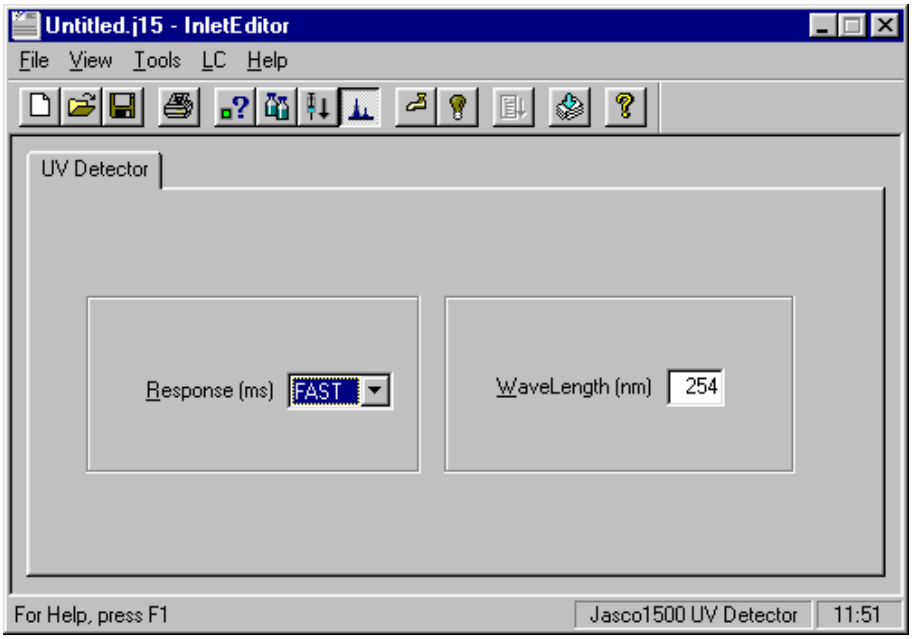


Figure 6.4 *UV Detector Configuration page*

Response This can be set to Fast, Standard or Slow depending on the length of time you expect the peak to appear.

Wavelength Set to the wavelength you want to monitor.

Notes

Notes

Shimadzu Systems

Chapter 7

Shimadzu Systems

Shimadzu Autosampler Initial Conditions Page

This page is used to set parameters specific to the Sampler, to access it select **Shimadzu AutoSampler** from the **View** menu or press the toolbar button.

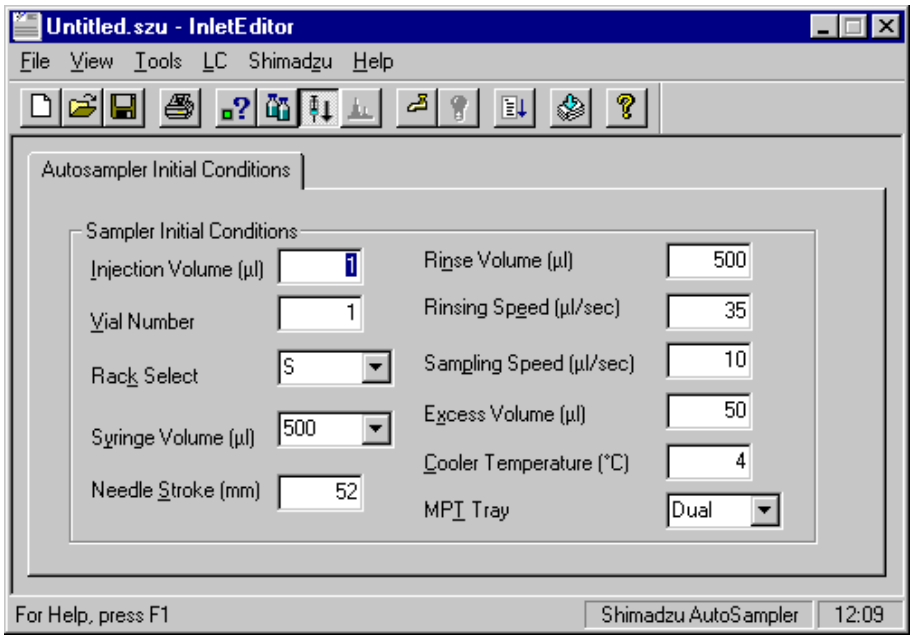


Figure 7.1 *Autosampler Initial Conditions page*

Injection Volume Enter the volume in microlitres to inject.

Note: If you are running from the Sample List, the injection volume in the sample list entry overrides the setting used here.

Vial number The vial to inject from.

Note: If a multisample acquisition is being run from the MassLynx Sample List, the Bottle # entry in the sample list overrides the value given in the Vial Number entry above.

Rack Select Select the type of rack required from the drop down list box.

Syringe Volume Select the size of the currently installed syringe from the drop down list box.

Needle Stroke Adjusts the depth of the needle tip to accommodate for sedimented samples or non-standard vials.

Rinse Volume Enter the volume of solvent that is to be rinsed through the needle.

Rinsing Speed Enter the speed at which the solvent is to be rinsed through the needle.

Sampling Speed Enter the rate in microlitres per second at which sample is extracted into the autosampler needle. This should be set according to the viscosity of your sample.

Excess Volume To ensure that the sample is not diluted with the rinse solvent more sample is drawn into the needle than will be injected. Enter the extra volume required.

Cooler Temperature If the sample cooler is installed, enter the temperature that the sample should to be cooled to.

MPT Tray Select Dual or Single from the drop down list box.

- **To Set-up Communication Parameters (Shimadzu)**

Select **Configuration** from the **Shimadzu** menu to display the Configuration dialog.

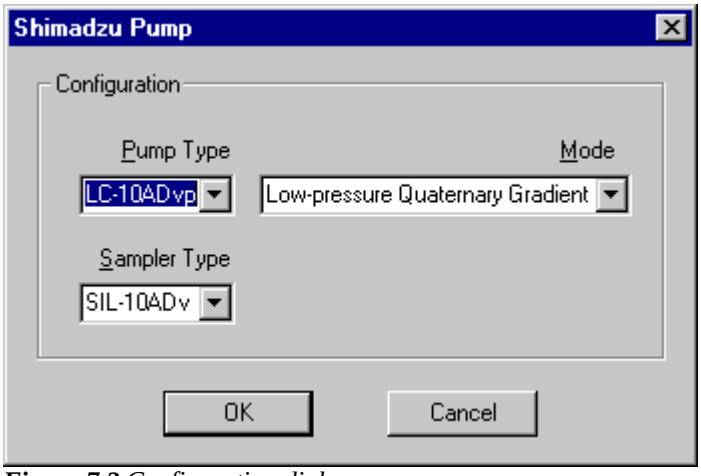


Figure 7.2 *Configuration dialog*

These parameters should be defined on setup and should only need changing if the Pump, Autosampler or mode of acquisition is changed. To change a value select a new one from the relevant drop down list box.

Shimadzu Pump

The Shimadzu Pump pages can be accessed by selecting **Shimadzu Pump** from the **View** menu on the Inlet Editor or by pressing the  toolbar button.

- **Shimadzu Initial Conditions Page**

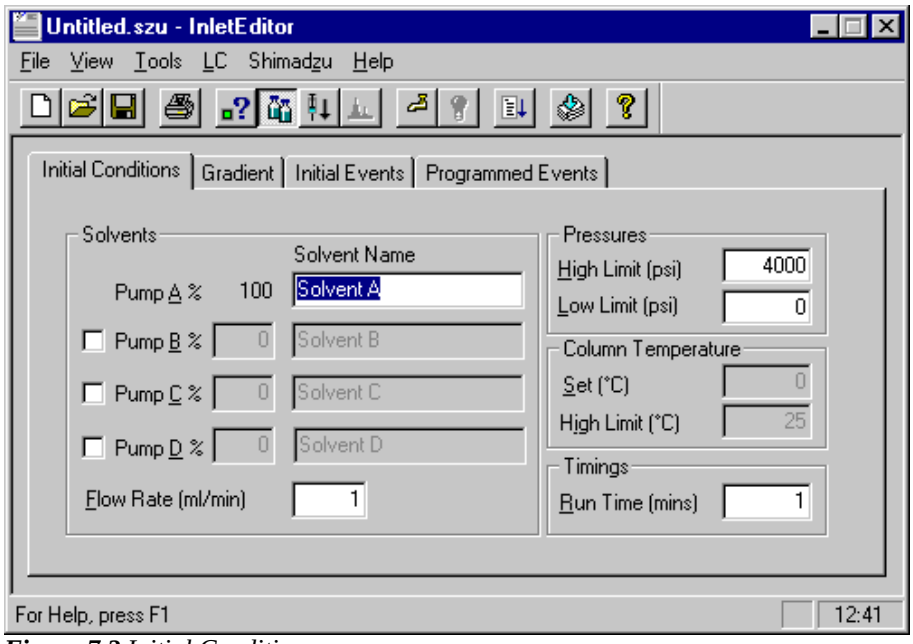


***Figure 7.3** Initial Conditions page*

Solvents Up to four solvents will be displayed depending upon the system configuration. The total value of all the solvent percentages added together must not exceed 100%.

Pump A This is the remainder percentage after the solvent percentages have been set for the other pumps.

Pump B, C and **D** These can either be enabled or disabled by checking the box next to the individual pumps. The values can be set to the required percentage of flow delivery.

Flow Rate This is the total flow rate of the solvent channels according to how you have configured the instrument.

Enter **High Pressure Limit** and **Low Pressure Limit** values as required. If the pressure falls outside these limits the current acquisition will stop and the LC Status error light, on the MassLynx screen, will turn red.

Column Temperature Set Enter the temperature to heat the column to. **Note:** This box will be greyed out if a column heater is not present.

Column Temperature High Limit This is the maximum deviation in column temperature allowed. If this is exceeded the current acquisition will stop and the LC Status error light, on the MassLynx screen, will turn red.

Run Time Enter the time in minutes that the method will run from the point of injection.

Shimadzu Gradient Timetable Page

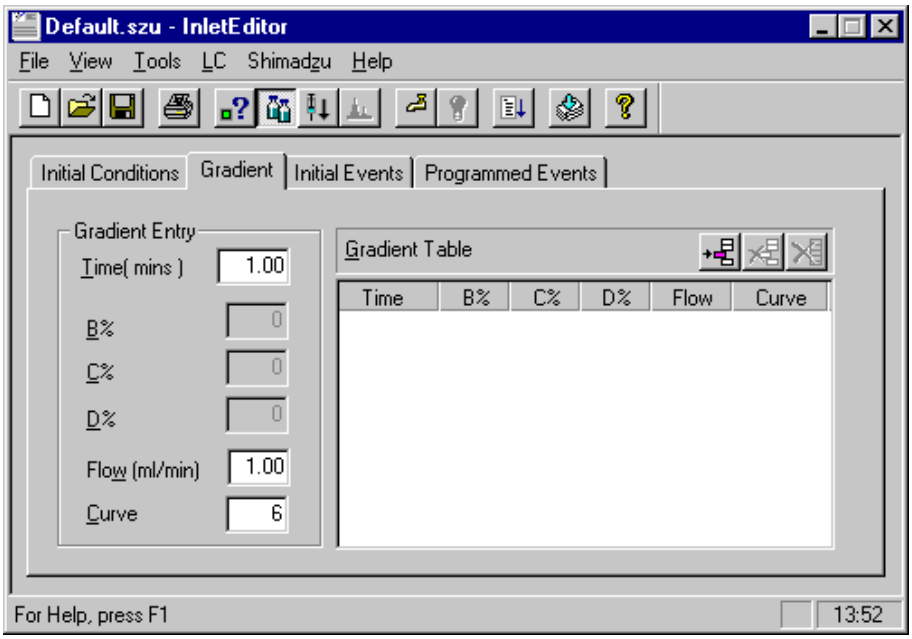


Figure 7.4 *Gradient Timetable page*

This page allows a gradient to be entered and edited. To operate in isocratic mode ensure that the timetable is empty.

To add a gradient, enter a time and percentage in the relevant boxes and press the  toolbar button. **Note:** The first entry must have a time of 0.

To delete a single gradient click with left mouse button on a time in the list and press the  toolbar button.

To delete all entries press the  toolbar button. This button is only available when there are entries in the timetable.

To modify a gradient select the required entry in the timetable. The values will then be displayed in the edit boxes above the timetable, and can be altered as appropriate. Once changed press  to re-enter the values into the timetable. If, however, you modify the time value such that it does not correspond to any existing entry in the timetable pressing  will result in a new entry being created in the timetable.

Flow Enter the flow rate for the solvent delivery system.

Curve This sets the rate at which the solvent is to change to the new proportions and/or flow rates. See the Shimadzu Operator's Guide for a list of values.

- **Shimadzu Initial Events Page**

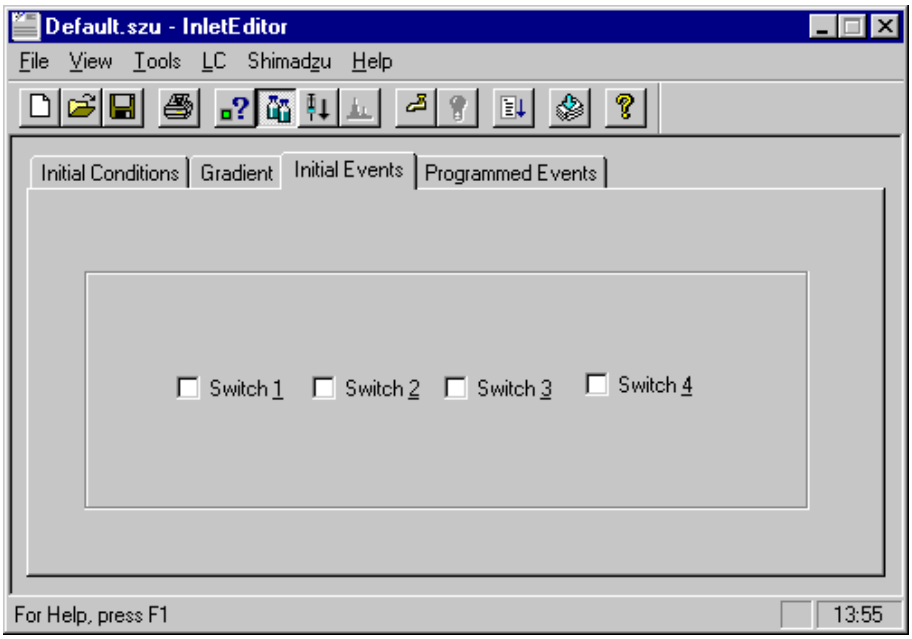


Figure 7.5 *Initial Events page*

This page allows the initial state of switches 1 to 4 to be defined. Check the box(es) for the switches that should have an initial state of off.

Shimadzu Programmed Events Page

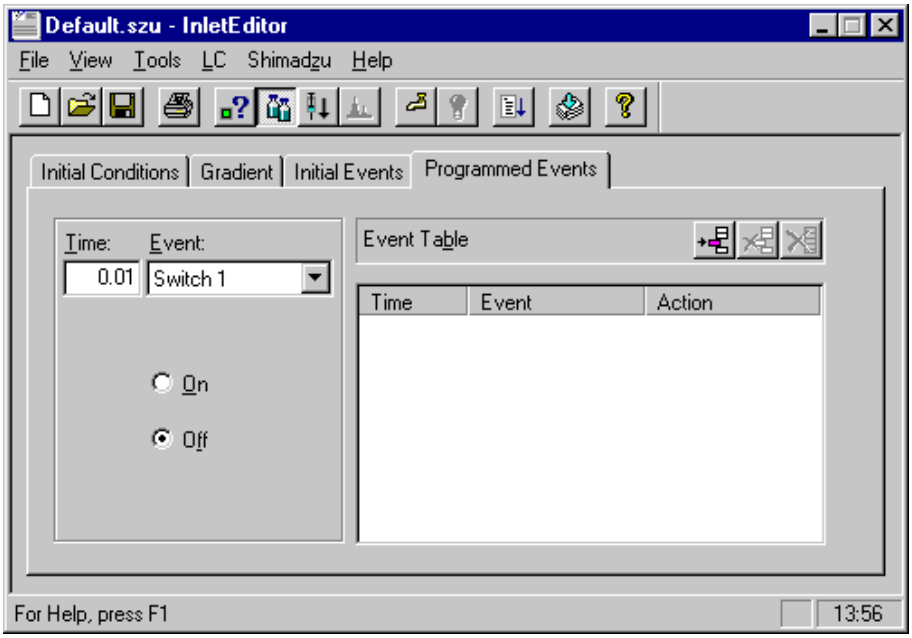


Figure 7.6 *Programmed Events page*

This page allows the state of switches 1 to 4 to be programmed.

To add an event, enter a time, select an event from the drop down list box, select an action (**on** or **off**) and press the  toolbar button.

To delete a single event, click with left mouse button on a time in the list and press the  toolbar button.

To delete all entries press the  toolbar button. This button is only available when there are entries in the timetable.

To modify an event, select the required entry in the timetable. The values will then be displayed in the edit boxes above the timetable, and can be altered as appropriate. Once changed press  to re-enter the values into the timetable. If, however, you modify the time value such that it does not correspond to any existing entry in the timetable pressing  will result in a new entry being created in the timetable.

Notes

Notes

CTC, Cetac and Other Systems

Chapter 8

CTC A200S Autosampler

These pages are used to set parameters specific to the Sampler, to access them select **CTCA200S AutoSampler** from the **View** menu or press the  toolbar button.

- **CTC A200S Status Page**

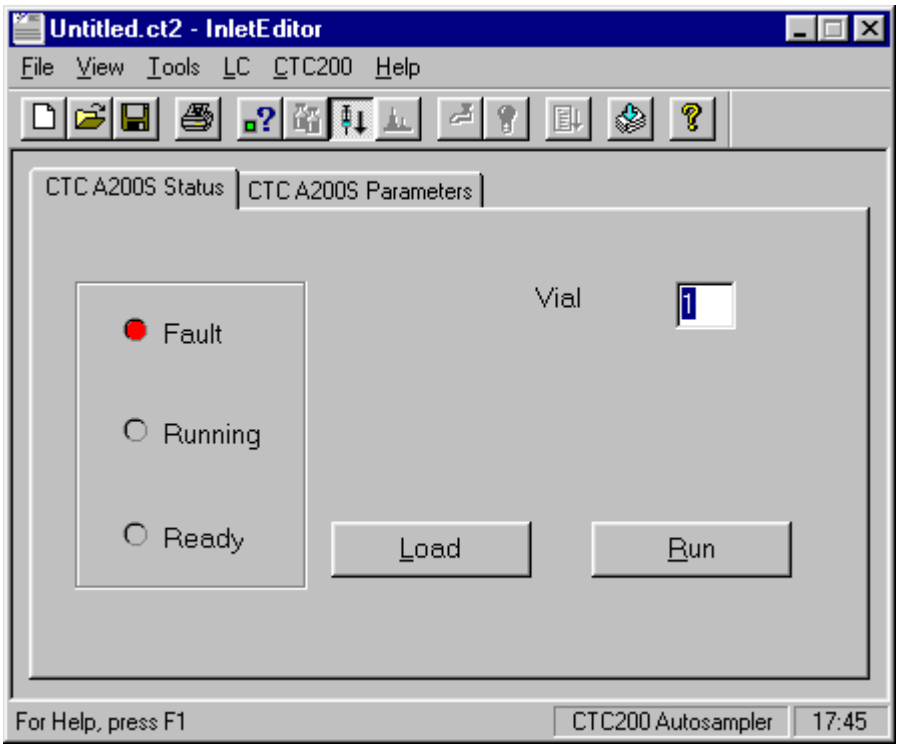


Figure 8.1 *CTC A200S Status page*

The Fault, Running and Ready indicators at the left side of the screen give information on the current status of the autosampler.

Indicator	Red	Green
Fault	Fault with the autosampler	No fault
Running	Not running	Running
Ready	Not ready	Ready

Vial Enter the number of the vial to take the sample from, for a single injection.
Note: When samples are acquired from the Sample List the number on the Sample List overrides this value.

Press the Load button to download the parameters to the LC system.

Pressing the button or choosing **Load Method** from the **LC** or **CTC200** menu will perform the same action.

Press the Run button to run a single injection. Pressing the button or choosing **Run Method** from the **LC** or **CTC200** menu will perform the same action.

- **CTC A200S Parameters Page**

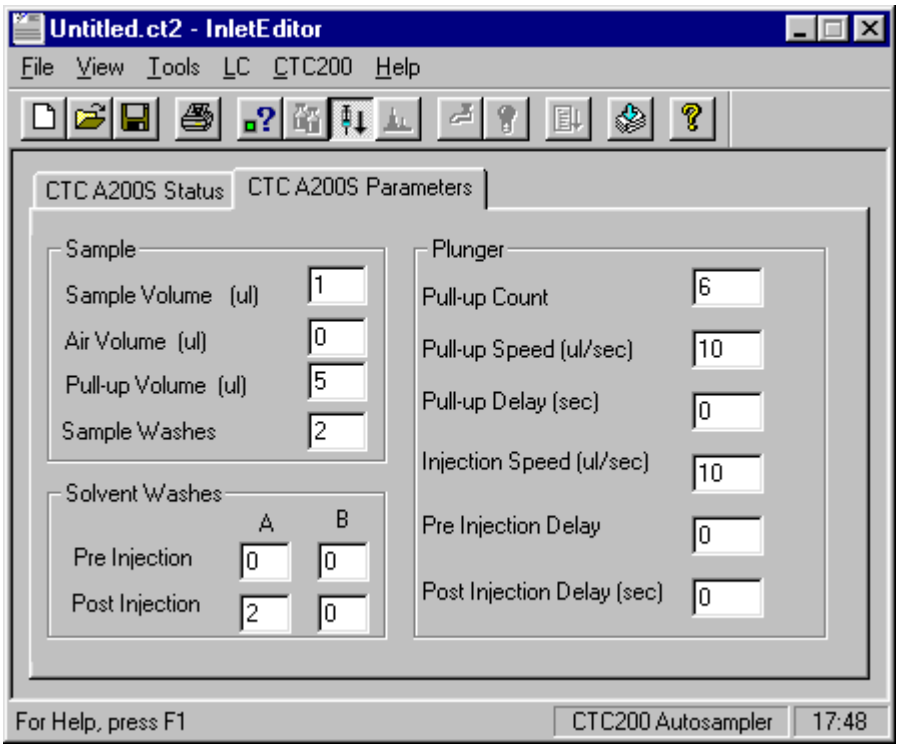


Figure 8.2 *CTC A200S Parameters page*

Sample Volume Enter the volume of sample (in microliters) to inject.

Air Volume Enter the volume of air (in microliters) to be drawn into the needle before the sample, to separate it from the previous sample.

Pull-up Volume Enter the volume of sample (in microliters) to draw into the needle for a sample wash.

Sample Washes Enter the number of times to wash the needle with sample.

Solvent Washes Pre Injection Enter the number of solvent washes to perform using solvent from reservoirs A and/or B, before an injection.

Solvent Washes Post Injection Enter the number of solvent washes to perform using solvent from reservoirs A and/or B, after an injection.

Pull-up Count Enter the number of times to pull up the Pull-up volume for a sample wash.

Pull-up Speed Enter the speed (in microliters per second) to pull up the Pull-up volume for a sample wash.

Pull-up Delay Enter the time to wait between each pull up.

Injection Speed Enter the speed (in microliters per second) to inject the sample.

Pre Injection Delay Enter the time to wait (in seconds) between the needle being injected and the plunger being depressed.

Pre Injection Delay Enter the time to wait (in seconds) for the plunger to be drawn back after an injection.

CTC PAL Autosampler

These pages are used to set parameters specific to the Sampler, to access them select **PAL_CC AutoSampler** from the **View** menu or press the  toolbar button. When the autosampler parameters are selected the following message is displayed.

Figure 8.3 *Error message*

This refers to the Macro Editor, which is not part of the standard Cycle Composer software, see the PAL Cycle Composer User Manual for details. Press the **Cancel** button to proceed.

When the software is installed a series of files are copied to the default.pro/Acqudb directory (*.pma and *.pol).

When the autosampler page is selected the software looks for the presence of the PAL autosampler. If one is found information is read from the Latest_pal.pol file.

To create method editor files when not connected to a PAL copy the Offline_pal.pol file to the Acqudb directory of the required project. When complete, copy the Method files (*.ccp) to the Acqudb directory of the required project on the acquisition PC.

PAL Cycle Composer Method Editor

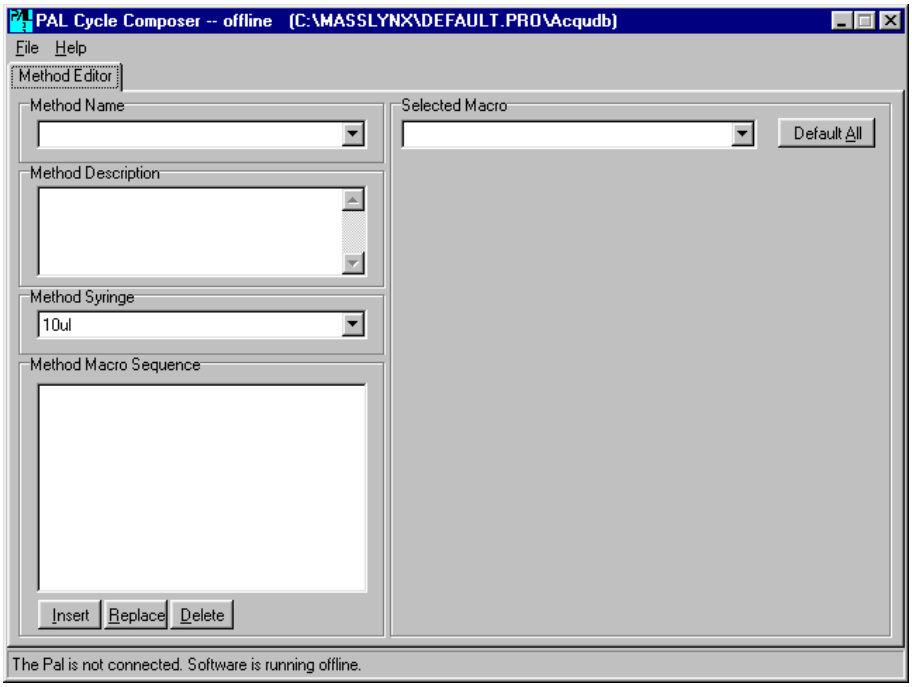


Figure 8.4 *Pal Cycle Composer Method Editor dialog*

To Create a Method (CTC PAL)

1. Select **New Method** from the **File** menu. The **Choose name of new Method** dialog is displayed.

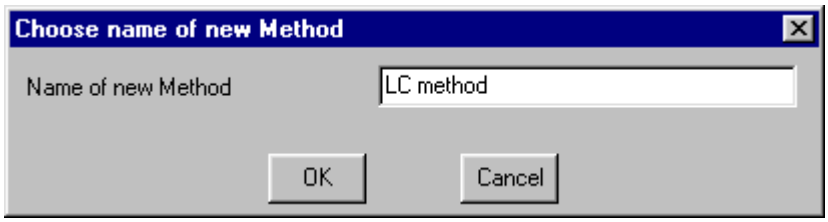


Figure 8.5 *Choose name of new Method dialog*

2. Enter the name for the method and press **OK**.

3. Enter a description of the method in the **Method Description** box.

4. Select the size of the syringe installed from the **Method Syringe** drop down list box.

   Note: The syringe size should be defined before any macros are selected as different default values and ranges are defined for each syringe size. Changing the syringe size after selecting macros could result in the values entered being outside the ranges allowed and so the macro values will have to be adjusted.

5. Select a macro from the **Selected Macro** drop down list box. The parameters required for the macro are displayed below the selected macro box.

   Note: Placing the cursor on the macro name will display a short description of the macro function, as in **Figure 8.6**.

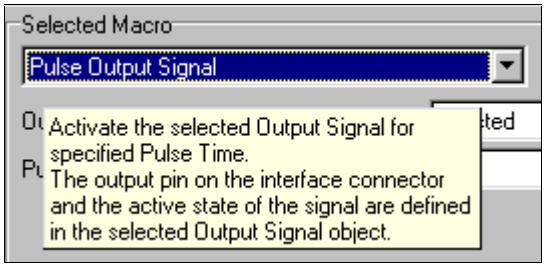


Figure 8.6 *Macro description*

Placing the cursor on a field will display a description of the valid values for this field, as in **Figure 8.7**.

Figure 8.7 *Macro description*

6. When the parameters for the macro have been entered press the **Insert** button and the macro will be added to end of the list in the **Method Macro Sequence** box.

   To replace a macro, click with the left mouse button on the macro in the **Method Macro Sequence** box, select the macro to replace it with, define the required values and press the **Replace** button.

   To remove a macro from the list, click with the left mouse button on the macro in the **Method Macro Sequence** box and press the **Delete** button.

7. Select **Save Method** or **Save Method As** from the **File** menu. The **Save Method** dialog is displayed with the name defaulted to that entered in step 2. The name can be changed if required, any changes made will be reflected in the **Method Name** in the editor. Press the **OK** button to save the method.

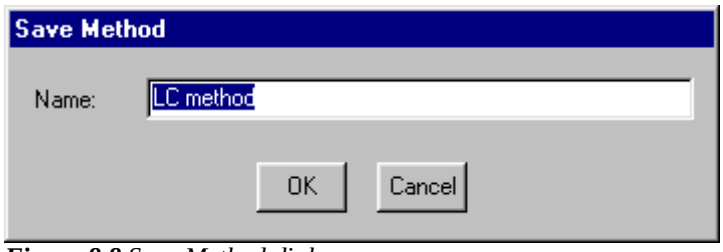


Figure 8.8 *Save Method dialog*

8. The method file (*.ccp) is stored in the Acqudb directory of the current project.

To Modify a Method (CTC PAL)

1. Select the method required from the **Method Name** drop down list box. The method files (*.ccp) displayed are those stored in the Acqudb directory of the current project.

2. Click with the left mouse button on the required macro in the **Method Macro Sequence** list and change the parameters displayed on the right of the dialog.

   Note: If the syringe size is changed macro values will have to be adjusted as different syringe sizes have different field values.

3. To add a macro, select the macro from the **Selected Macro** drop down list box. The parameters required for the macro are displayed below the selected macro box.

   When the parameters for the macro have been entered press the **Insert** button and the macro will be added to end of the list in the **Method Macro Sequence** box.

   To replace a macro, click on the macro in the **Method Macro Sequence** box, select the macro to replace it with, define the required values and press the **Replace** button.

   To remove a macro from the list, click on the macro in the **Method Macro Sequence** box and press the **Delete** button.

4. Select **Save Method** or **Save Method As** from the **File** menu. The **Save Method** dialog is displayed with the name defaulted to that entered in step 2. The name can be changed if required, any changes made will be reflected in the **Method Name** in the editor. Press the **OK** button to save the method.

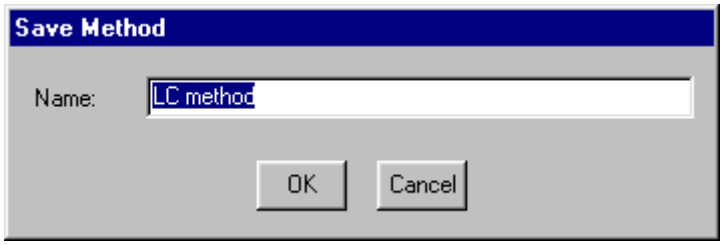


Figure 8.9 *Save Method dialog*

5. The method file (*.ccp) is stored in the Acqudb directory of the current project.

To Delete a Method (CTC PAL)

1. Select the method required from the **Method Name** drop down list box.

2. Select **Delete Method** from the **File** menu and press Yes on the confirmation dialog.

   Note: Methods can also be deleted using Window Explorer. Method files (*.ccp) are stored in the Acqudb directory of the current project.

Sample List Vial Referencing (CTC PAL)

For the CTC PAL autosampler the default Sample List vial referencing for a 96 well plate in Stack 1 is

Stk1-01:1 to 96 for the first tray in stack 1
Stk1-02:1 to 96 for the second tray in stack 1 etc.

I.e. Stk1-01:1 is entered in the SAMPLE_LOCATION (Bottle) column of the Sample List. To use the normal MassLynx referencing 1:1, 1:2, 2:1 etc. the trays have to be renamed. See page 179 for details.

Note: For OpenLynx the 1:1 tray:vial referencing must be used.

Using the PAL CTC Autosampler with OpenLynx

When using the CTC PAL autosampler with OpenLynx the tray names must be defined numerically and in sequence.

Note: It is recommended that MassLynx is closed down whilst changes are made to the tray numbering. When MassLynx is restarted the changes will be picked up automatically.

To Rename Trays (CTC PAL)

Using the hand held controller, check the order of the tray holders.

Using the hand held controller, number the trays for the tray holders sequentially starting from 1.

E.g. if the tray holders are in the order:

Stack1
THldr1

Then the trays should be numbered starting at 1 for the first tray in stack 1 and continuing sequentially for THdr1 trays (see the example in **Table 8.1**).

Tray Holder	Tray Type	Default Tray Name	OpenLynx Tray Name
Stack1	MT96	Stk-01	1
Stack1	MT96	Stk-02	2
Stack1	MT96	Stk-03	3
Stack1	MT96	Stk-04	4
Stack1	MT96	Stk-05	5
Stack1	MT96	Stk-06	6
Stack1	MT96	Stk-07	7
Stack1	MT96	Stk-08	8
Stack1	MT96	Stk-09	9
Stack1	MT96	Stk-010	10
Stack1	MT96	Stk-011	11
Stack1	MT96	Stk-012	12
THldr1	VT98	THldr-01	13
THldr1	VT78	THdlr-02	14

Table 8.1 *OpenLynx Tray Naming*

To check that trays are numbered correctly select **OpenLynx Plate Login** from the **Inlet Editor**, **Plate Login** menu.

If the trays are correctly numbered then the dialog will appear as in **Figure 8.10**. If the numbering is incorrect i.e. trays for THdlr1 are numbered from 1 then the dialog will appear as in **Figure 8.11**.

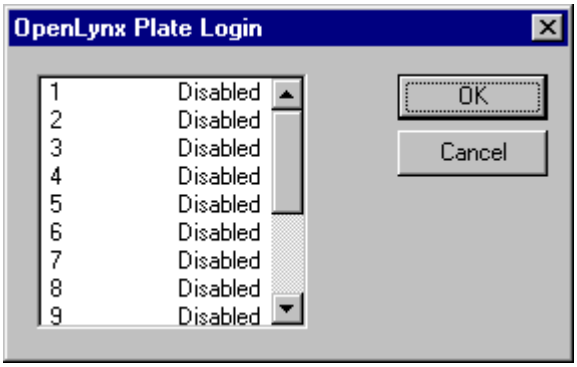


Figure 8.10 *OpenLynx Plate Login dialog*

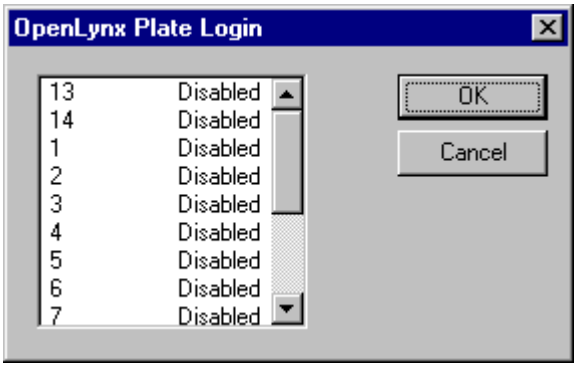


Figure 8.11 *OpenLynx Plate Login dialog*

- **Using Plates for OpenLynx Plate Login (CTC PAL)**

Select **OpenLynx Plate Login** from the **Inlet Editor**, **Plate Login** menu.

If a plate is labelled **Disabled** it can be used for single shot login. If a plate is labelled **Enabled** it can be used for plate login. To change the state double click on the tray number.

Cetac ASX100 Autosampler

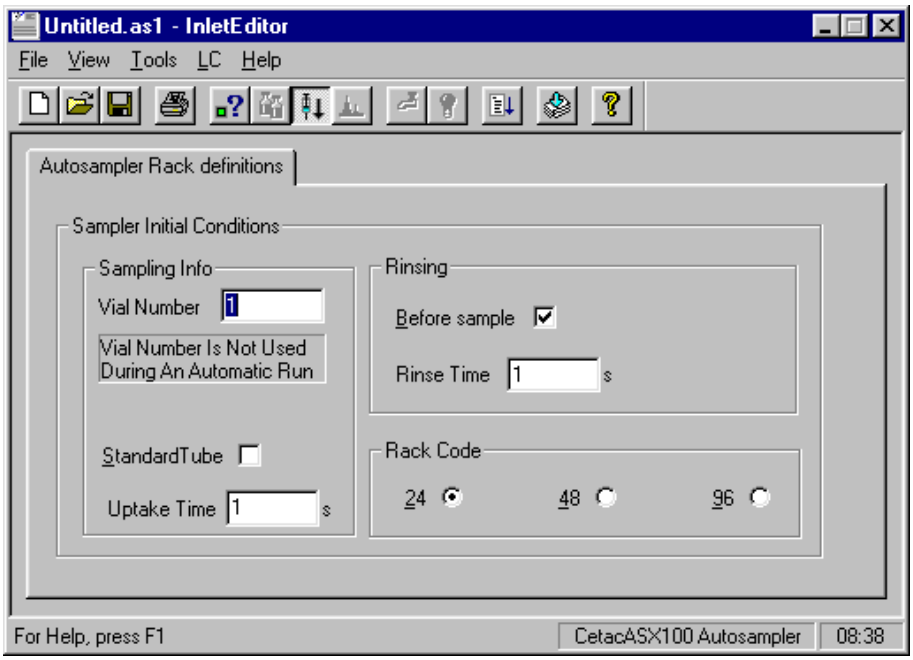


Figure 8.12 *Cetac ASX100 Setup dialog*

Technical details of this autosampler are to be found in the manual supplied with the Cetac ASX 100 autosampler.

Vial Number Enter the number of the vial to take the sample from. **Note:** When samples are acquired from the Sample List the number on the Sample List overrides this value.

Standard Tube Check this box if standard vials are being used. The rack codes section will be grayed out and vial number can only be 2 to 14.

Uptake Time Enter the time in seconds for the sample to travel from the sample vial to the Mass Spectrometer.

Before Sample Check this box to rinse the needle before each sample.

Rinse Time Enter the time in seconds required to rinse the needle.

Rack Codes Click with the left mouse button on the code required for the rack.

Cetac ASX500 Autosampler

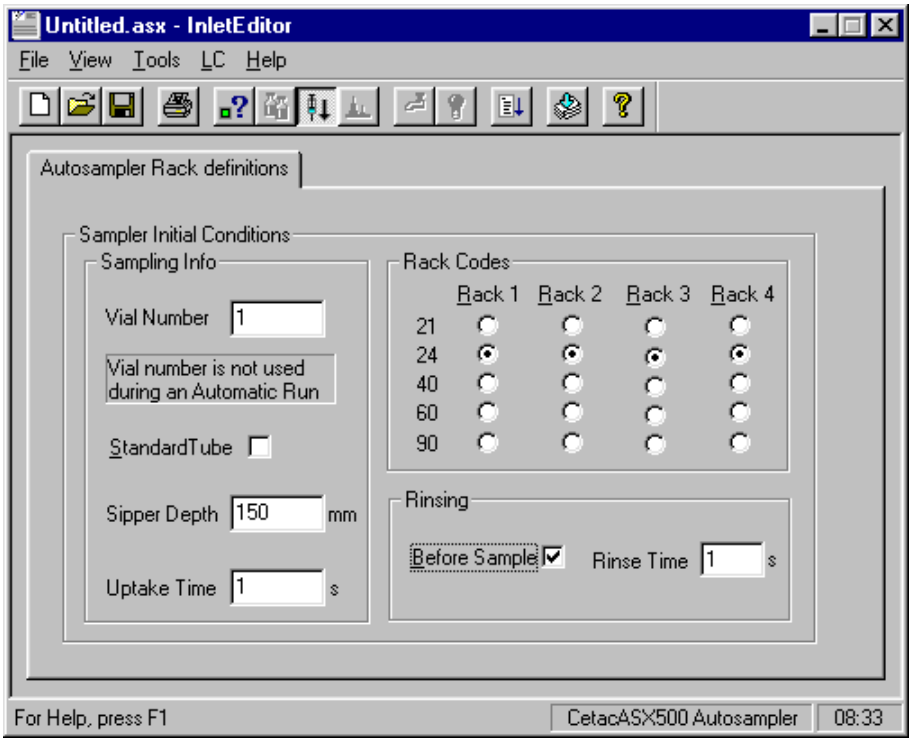


Figure 8.13 *Cetac ASX500 Setup dialog*

Technical details of this autosampler are to be found in the manual supplied with the Cetac ASX 500 autosampler.

Vial Number Enter the number of the vial to take the sample from. **Note:** When samples are acquired from the Sample List the number on the Sample List overrides this value.

Standard Tube Check this box if standard tubing is being used. The rack codes section will be grayed out and vial number can only be 1 to 10.

Sipper Depth Enter the depth in millimeters the needle should travel to.

Note: The default probe sampling depth is measured from the neck of the tube to the tip of the probe.

Uptake Time Enter the time in seconds for the sample to travel from the tubing to the Mass Spectrometer.

Rack Codes Click with the left mouse button on the code required for each rack.

Rinse Before Sample Check this box to rinse the needle before each sample.

Rinse Time Enter the time in seconds required to rinse the needle.

Solids Probe

The temperature of a solids probe can be controlled during an acquisition. To do this you must set a ramp that defines the temperature of the probe tip against retention time. The ramp can have up to 5 'segments' which each have a start temperature, a time for which the probe will be held at that temperature, and a rate at which the probe will be heated to reach the start temperature of the next ramp segment (if there is one).

In addition to these controls, TIC (Total Ion Current) control of the probe is also available. If TIC control is selected then the TIC value is monitored during the acquisition and that information is used to modify the programmed ramp in such a way that the system attempts to keep the TIC at or below the 'Maximum TIC' value. This feature is very useful as it stops samples from being 'burnt off' the probe prematurely.

The actual temperature ramp used can be stored with the data file and a remote contact closure can be used to start the ramp. The **External Contact Start** box should be checked when a robotic probe system is being used.

To Change probe control parameters (Solids Probe)

1. Choose **Inlet** from the Acquisition Control Panel **Methods** menu

   -or-

   Double click on the probe icon on the Acquisition Control Panel to bring up the solids probe editor shown below.

2. Make any changes to the parameters.

3. Save the method using either **Save** or **Save As** from the File menu.

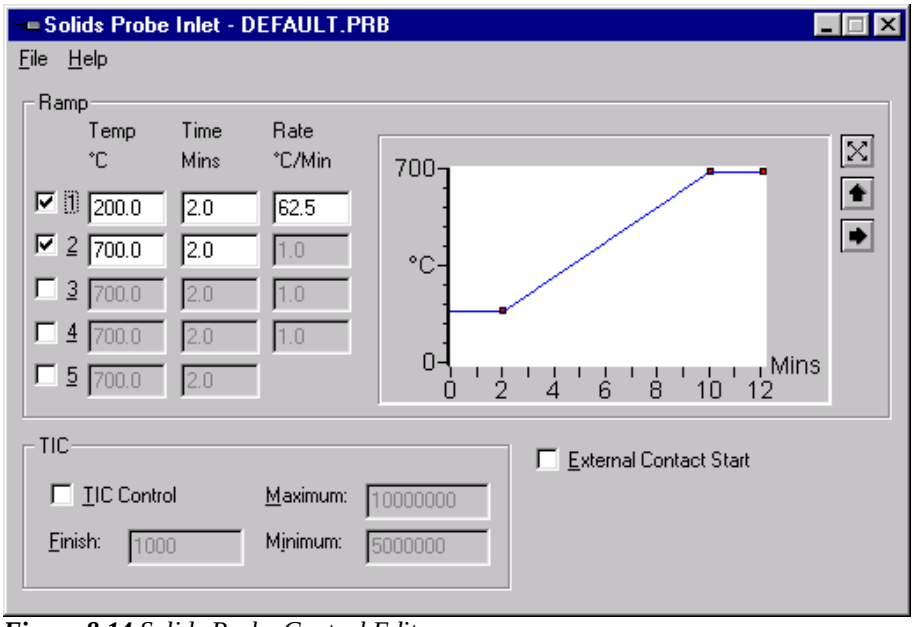


Figure 8.14 *Solids Probe Control Editor*

- **Programming the temperature ramp (Solids Probe)**

  The probe temperature ramp can be programmed using the keyboard or by dragging the small red handles on the picture of the ramp itself.

- **Using TIC Control (Solids Probe)**

  To use the TIC control feature you must first check the **TIC Control** box, which will enable the values in the TIC control group to be modified. There are 3 values that you then need to set.

  Minimum sets the value for the TIC above which the probe ramping is reduced. If the actual TIC seen from the instrument is below this value, the full heating rate, as programmed into the temperature ramp is used to heat the probe. As the TIC rises above this value, the heating rate is linearly adjusted down based on the difference between this minimum value and the maximum value discussed next. For example, a TIC value exactly between the maximum and minimum values would give a 50% rate compared to that requested by the ramp parameters.

  Maximum sets the value for the TIC at which the probe ramping is suspended. This is done because the system is trying to keep the TIC at this level and further heating would cause it to rise above it. If the TIC reaches this level, heating will not recommence until it falls back down below.

  Finish sets a value for the TIC below which the acquisition of data will terminate. The temperature program will continue however to allow any remaining sample to be burnt off.

DCI Probe

A DCI probe can be controlled in the same way as a solids probe, as described above with the exception that the ramp is programmed for Current rather than temperature and the DCI current can be stored with the data file, not the probe temperature.

Thermospray Probe

A thermospray probe can be controlled in the same way as a solids probe, as described above, with the exception that the thermospray nozzle temperature can be stored instead of the probe temperature.

RoboProbe

A robotic probe system can be used in conjunction with a CE Instruments A200S auto injector, or a Zymark laboratory robot.

- **CE Instruments A200S**

  If the A200S is used then setting it up is done as described earlier.

- **Zymark Labmate**

The Zymark setup editor allows you to select a solvent for your sample.

1. Choose **Inlet** from the Acquisition Control Panel **Methods** menu

   or

   Double click on the Picture of the auto injector on the Acquisition Control Panel to bring up the Zymark editor shown below.

2. Make any changes to the parameters.

3. Save the method using either **Save** or **Save As...** from the File menu.

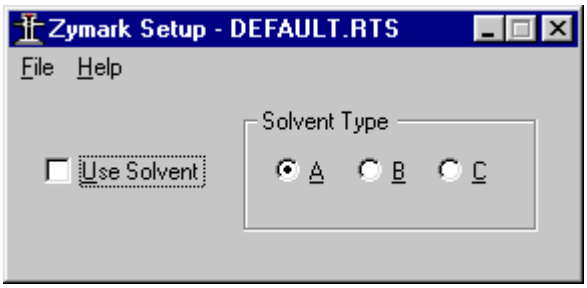


Figure 8.15 *Zymark Solvent Selection Editor*

Contact Closure

Contact closure is a common method of providing start/stop control of an external inlet system. Many chromatographs, both LC and GC support contact closure because it is often used to provide control of an integrator unit. MassLynx uses essentially the same method of synchronisation for acquiring data, the mass spectrometer's control unit using the start and stop signals produced by the chromatography system to start and stop data acquisition.

Notes

Notes

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