



02134

Omnion 3.0 Software

USER MANUAL

June 2006, Edition 3

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Section 1 Introduction

Due to a wide variety of available computers, operation of this software with a QuikChem 8000 or QuikChem 8500 is only guaranteed if the computer system is purchased from Lachat Instruments or successfully tested by Lachat Instruments.

1.1 Recommended system configuration

- Pentium 4 Processor, 1.6 GHz or higher
- 256 MB RAM
- 40 GB (or higher) Hard Drive
- CD-R/W, 3.5" Floppy Drive
- 17" Flat Panel Monitor
- Sound Card and Speakers (QuikChem 8500)
- 2 RS232C Serial Ports (QuikChem 8000, for Sampler and DRD dilutor)
- USB 2.0 Ports (QuikChem 8500)
- Windows 2000 or XP

Note: For Windows versions prior to XP and 2000 (95, 98, NT and ME), power on the QC8500 instrument and verify connection to the PC before launching Omnion. If the USB connection to the instrument is lost (e.g. momentary interruption of power to the PC or QC8500 instrument due to power surges), reboot the PC to reestablish communication. (Windows 2000 and XP will prompt the user to recover the link without rebooting.) Lachat Instruments strongly recommends using Windows 2000 or Windows XP operating systems with the QC8500.

1.2 Minimum system requirements

- Pentium Processor, 600 MHz or higher
- 128 MB RAM
- 40 GB (or higher) Hard Drive
- CD-ROM, 3.5" Floppy Drive
- 15" CRT Monitor (1024x768 minimum)
- RS232C Serial Port (QuikChem 8000)
- USB Port (QuikChem 8500 or QuikChem 8000 with National Instruments 4350 USB device)
- 98SE, NT 4.0

Section 2 Installation

Note: For detailed software installation instructions, refer to the *Omnion Installation Instructions, Part No. 85259*.

For the QuikChem 8000, Omnion 3.0 installation is a 2-step process; installing the software and installing the I/O module. The QuikChem 8500 does not require an I/O Module.

2.1 Installing the software (QuikChem 8000 and QuikChem 8500)

2.1.1 Installing from CD-ROM

Insert the Omnion 3 CD into the CD-ROM drive and follow the instructions from the Omnion 3 Installation Guide.

Note: To obtain a copy of the *Omnion 3 Installation Guide*, contact Lachat Technical Support.

2.1.2 Running Omnion FIA or IC v 2.0 after upgrading (QuikChem 8000)

The Omnion 3.0 installation will not affect Omnion 2.0 FIA or IC. Both programs may be run for data analysis, using Windows 98. However, if the SS420 board(s) were removed or the operating system is upgraded to Windows 2000 or NT, new data on Omnion 2.0 cannot be acquired. Omnion 2.0 can still be accessed to review data. Omnion 2.0 IC requires a software key installed on the printer port in order to open the IC data files.

2.2 Installing the I/O Module (QC8000 only)

Important Note: Install software before installing boards.

Note: If the system unit has more than 4 channels, a second I/O module and communication cable is required. If more than one PCI board is required, install and run the Omnion software with the first board, then repeat for the second board, connecting its cables to JA2/JD2 on the system unit. Label the PCI boards as device 1 and device 2.

The I/O module is a plug-and-play device; no modifications to the board are required. When installed, it is automatically assigned an open IRQ level. The board is 17.5 cm (6.9 in.) long and 10 cm (3.9 in.) wide. The board is factory installed in all Lachat supplied computers.

1. Turn the computer off and remove the computer cabinet.
2. Remove the screws holding the slot cover plate behind the computer. Retain the screws.
3. Carefully remove the I/O module from its protective bag. To avoid damaging the card, use a grounding strap or discharge any static electricity that may have accumulated by touching the chassis of the computer before handling the board.
4. Plug the board into the appropriate PCI buss slot. Firmly push the edge of the board with the gold contacts into the PCI slot until the board is firmly seated.
5. Replace the slot cover plate using the slot cover plate screws. Secure the board in place by screwing it into the chassis through the hole at the end of the board (Figure 1).

6. Replace the computer cabinet and locate the A/D interface cable.
7. Plug the large Omnion 3.0 split cable into the rear of the I/O module.
8. Plug the analog cable into the port labeled JA1 and firmly tighten the screws to secure.
9. Plug the digital cable into the JD1 port, located below the analog cable. Firmly tighten the screws.

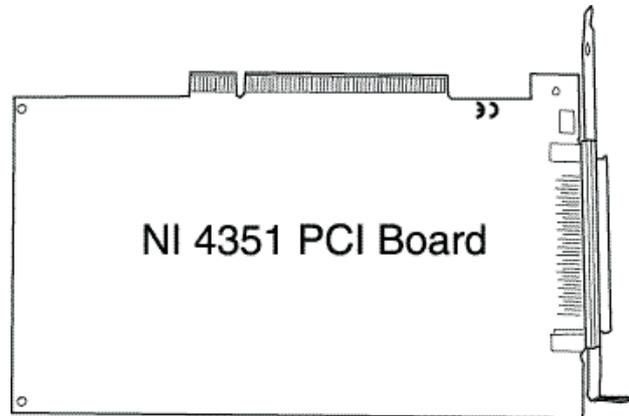


Figure 1 Omnion PCI board

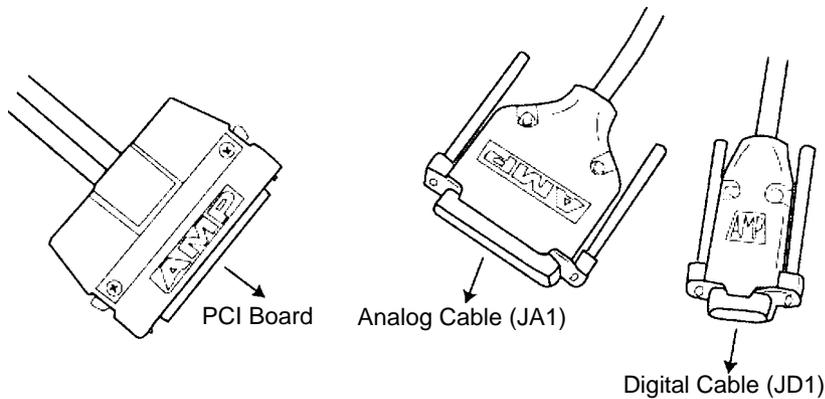


Figure 2 Communication cables

2.2.1 USB option

If the computer does not have an available PCI buss slot (i.e. laptop computers), a USB converter box can be used to interface the PCI board between the computer and system unit. The PCI board is installed in the converter box.

1. Plug the communication cable into the front of the converter box.
2. Plug the analog and digital cables into the respective ports.
3. Connect the USB cable to the rear of the interface box and to the USB port on the computer.

2.3 Upgrading hardware (switching from Omnion 2.0 to 3.0, QC8000 Only)

2.3.1 AIM 1250 autosamplers with DRD dilutors

Note: Only qualified personnel should perform the tasks described in this section. To schedule service, contact Lachat Instruments.

Omnion 3.0 communicates with the dilutor at 9600 baud, not 1200 baud as in Omnion 2.0. To prepare the DRD dilutor to run with Omnion 3.0:

1. Disconnect Power from the DRD Dilutor.
2. Open the dilutor chassis by removing the four screws from each side of the unit (eight screws total).
3. Locate the block of DIP switches (relays) labeled 1–8.
4. Set Switch 1 to the open position by pressing the bottom of the switch. All other switches must be in the closed position.

2.3.2 Gilson autosamplers

Omnion 3.0 will look for the Gilson Autosampler as Unit ID 0.

Section 3 QuikChem 8500 system configuration

3.1 Configuring the QuikChem 8500

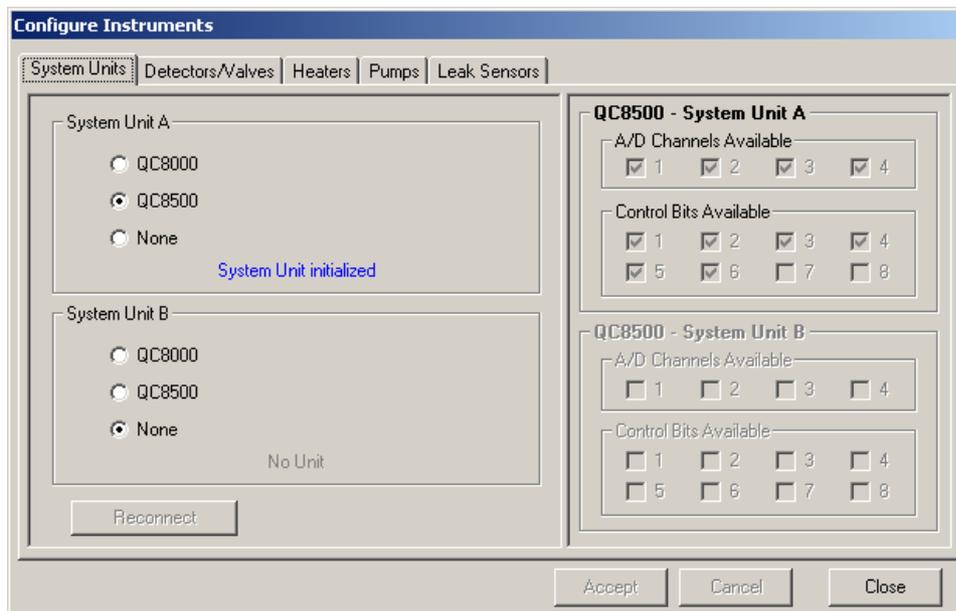
Note: Computers supplied by Lachat Instruments are factory-configured for QuikChem systems. Proceed to [Section 9, Run setup, on page 47](#). For all other computers, configure the system before proceeding with the Run Analysis.

Omnion software 3.0 version 219 and higher supports the QuikChem 8500 and the QuikChem 8000 (section [4.1 on page 19](#)) as individual systems. The software can also be configured for using both systems together (section [5.1 on page 23](#)).

3.1.1 QC8500 channel configuration

A single QuikChem 8500 can be configured for up to four channels. A second QC8500 is configured for five to eight channels.

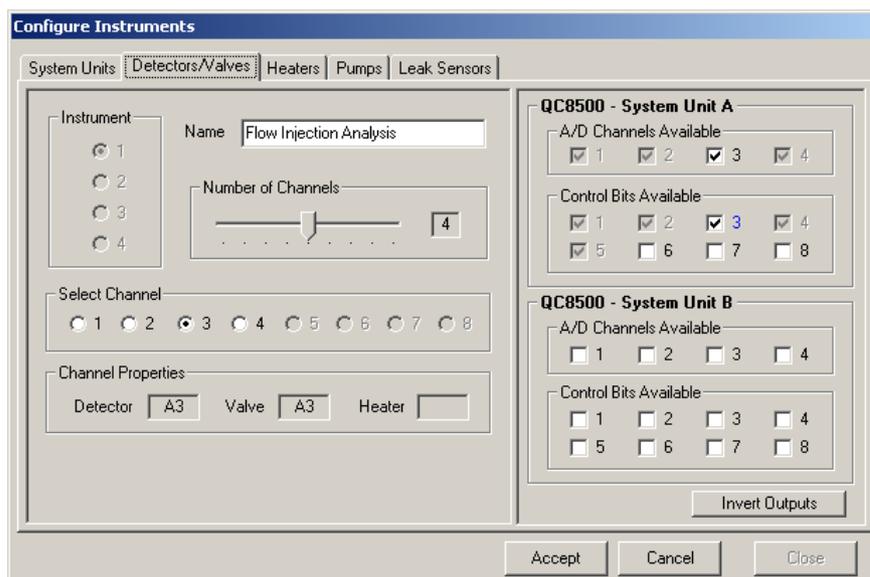
1. Start Omnion 3.0 software using the desktop icon or the Windows toolbar.
2. From the main menu, select **CONFIGURATION>INSTRUMENTS**.
3. Click the **System Units** tab. Select QC8500 as Device 1 for 1 to 4 channels. For 5 to 8 channels on the same computer, select QC8500 for both Device 1 and Device 2.



Note: A second QC8500 System Unit is required for operating 5 to 8 channels on one computer. Select the second QC8500 under System Unit B.

4. Click the **Detectors/Valves** tab.

- Enter the name of the run. For example, if the instrument was used to run a two-channel flow injection analysis measurement, a possible name is “Flow Injection Two-channel Instrument”.



- Drag the slider to the desired number of channels.
- Select the Channel number to configure. Each instrument channel can be configured individually.
- Select the position for the A/D channel and the control bit setting. (See [Table 1.](#))

Note: If the position is unavailable, verify that these resources are not currently being used with another instrument. Only one channel can use each A/D channel and control bit.

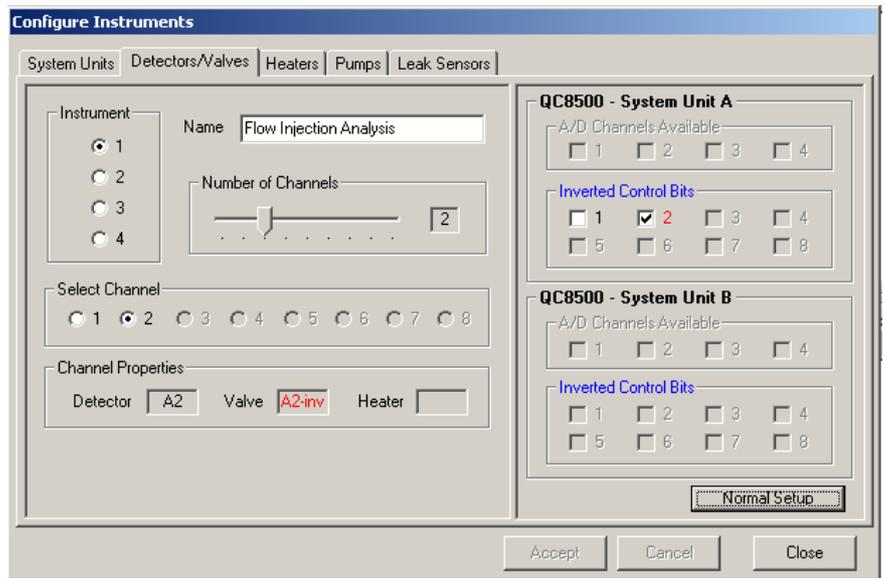
Table 1 Typical channel configuration (QC8500)

Parameter	System Unit A				System Unit B			
	1	2	3	4	5	6	7	8
Channel Number	1	2	3	4	5	6	7	8
A/D (Detectors)	1	2	3	4	1	2	3	4
Control Bit (Valves)	1	2	3	4	1	2	3	4

- Click **ACCEPT** to save changes. Click **CANCEL** to leave the configuration.

Follow steps 7–9 to configure additional channels.

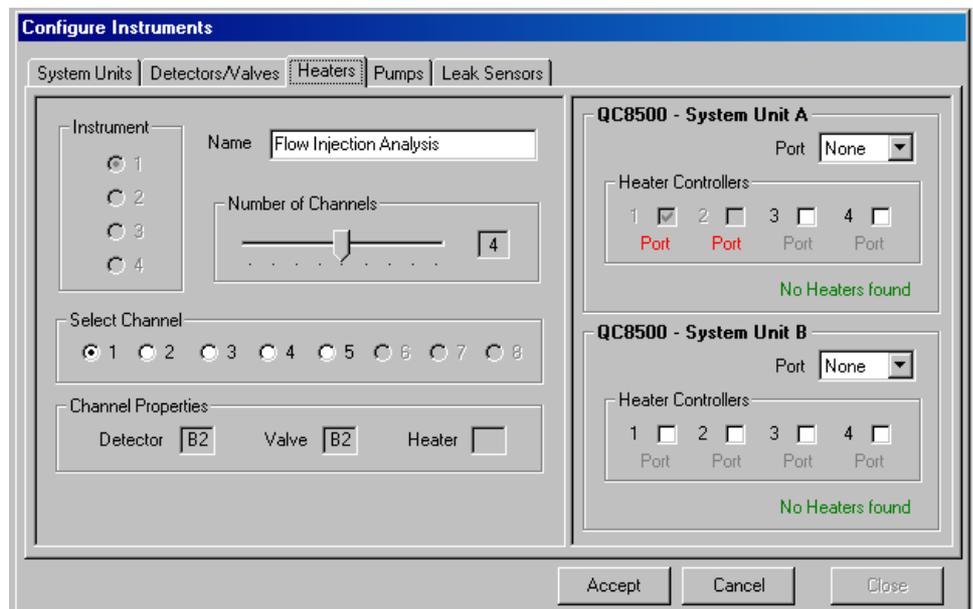
Important Note: For IC channels, the control bit outputs **MUST** be inverted to allow for proper configuration of the valve. To invert the control bit outputs, select the channel designated for IC. Click **INVERT OUTPUTS** and select the control bit to invert. Once selected, the inverted control bit number will turn red and the valve box under channel Properties will be red and show the valve state as inverted.



3.1.2 Heater configuration

Heater resources are configured as part of the instrument setup.

1. From the main menu select **CONFIGURATION>INSTRUMENTS**. See [Table 2](#) for typical configuration settings.
2. Click the **Heaters** tab to access the heater configuration screen.
3. Select the channel with the installed heater.



4. Select an available port for each heater in the Heater Controller section.
5. Press **ACCEPT**.

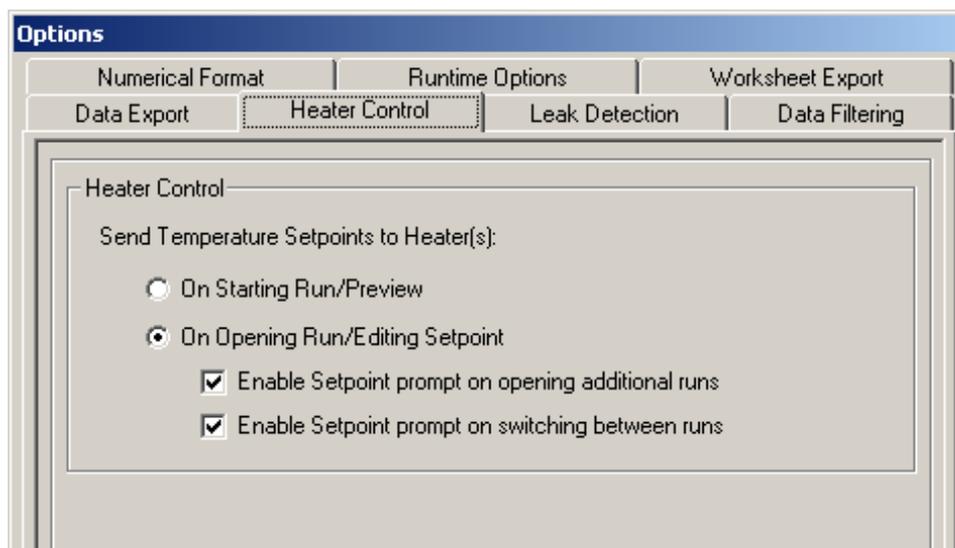
Table 2 Typical heater configuration (QC8500)

Parameter	System Unit A				System Unit B			
	1	2	3	4	1	2	3	4
Channel Number	1	2	3	4	1	2	3	4
Port Number	1	2	3	4	1	2	3	4

3.1.2.1 Setting the heater options

The heater can be set to warm up when a run is started or previewed, when a run is opened or when the set point is edited.

1. From the main menu, select **CONFIGURATION>OPTIONS**.
2. Click the **Heater Control** tab.



Note: The heater set point is set in the Analyte screen of the Run Properties dialog. See [Setting the run properties on page 50](#).

3. To begin heater warm-up when the run is started or previewed, select "On Starting Run/Preview".

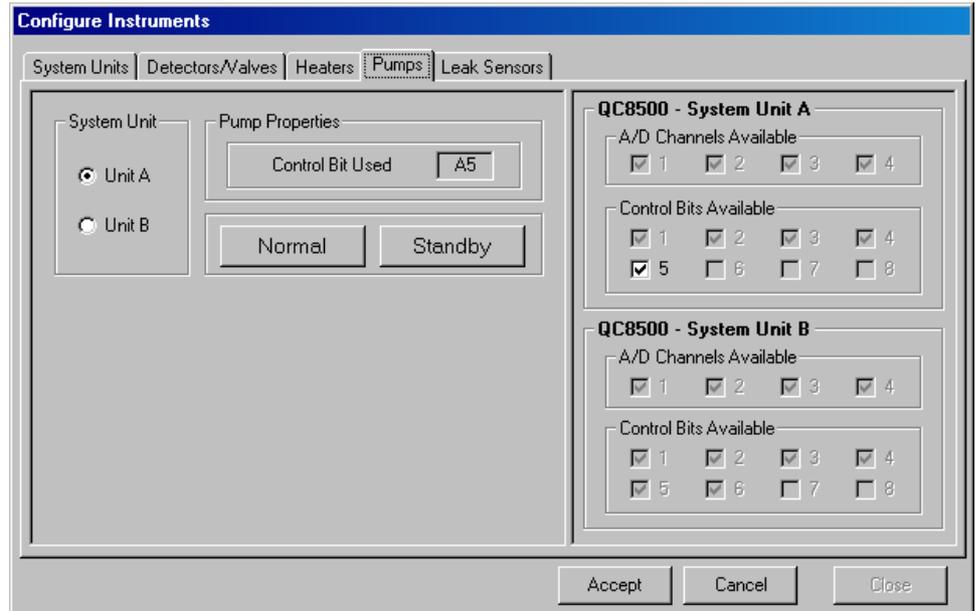
To begin heater warm-up when a run is opened or the set point is edited, select "On Opening Run/Editing Setpoint".

Prompts to start the heater when opening additional runs or switching between runs are enabled or disabled in this screen.

4. Click **ACCEPT**.
5. Click **CLOSE** to exit the Heater Control screen.

3.1.3 Pump control

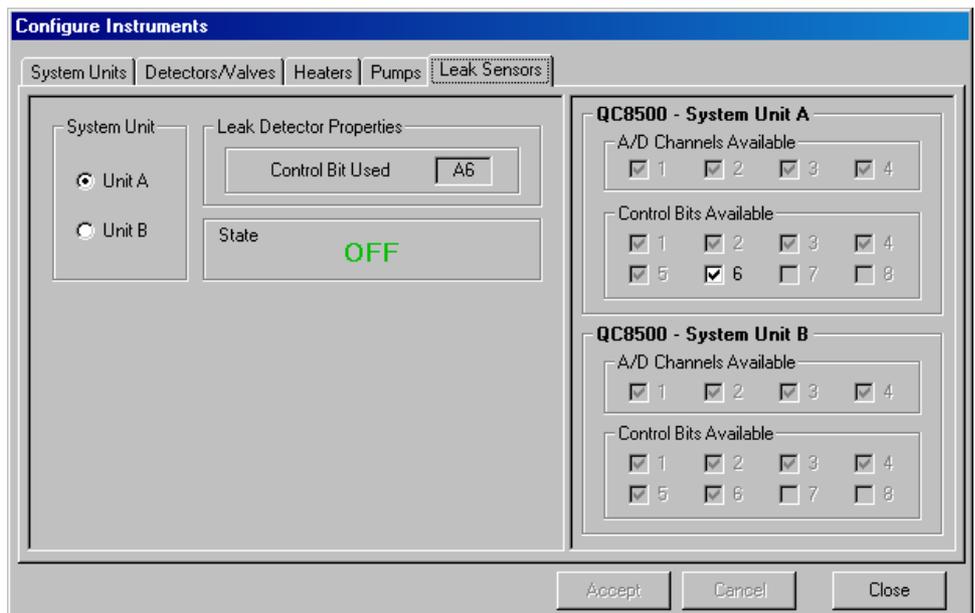
1. From the Main Menu, select **CONFIGURATION>INSTRUMENTS**. Click the **Pumps** tab.



2. Select System Unit A or B.
3. If necessary, change the speed of the pump to standby or normal speed.
4. Click **ACCEPT**, then **CLOSE**.

3.1.4 Leak sensor status

1. From the Main Menu, select **CONFIGURATION>INSTRUMENTS**. Click the **Leak Sensors** tab to access the leak sensor configuration screen.



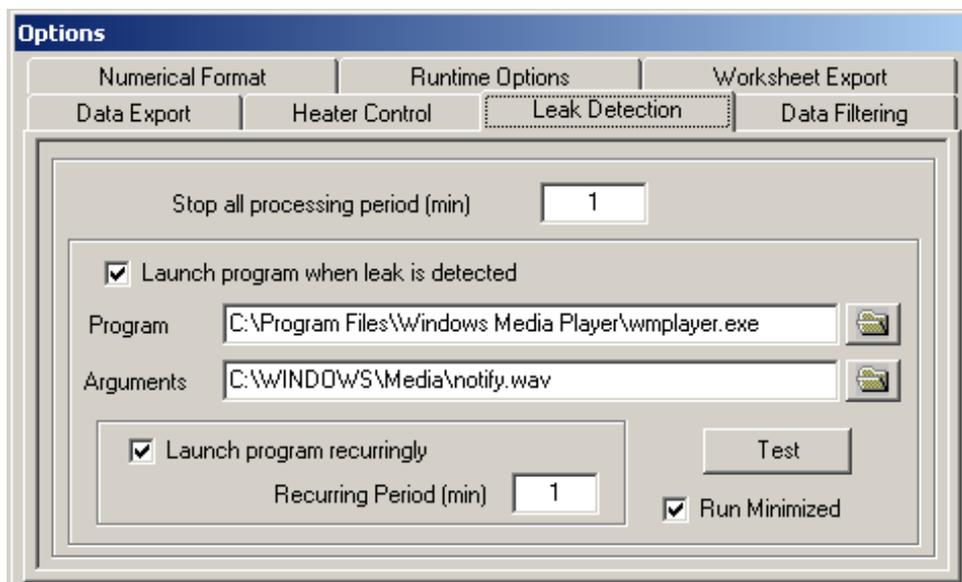
Note: The leak detection state is OFF when no leaks are detected.

2. Select System Unit A or B. Click **CLOSE**.

3.1.4.1 Setting the leak alarm

When a leak is detected, the system can be set to sound an alarm and to stop immediately, or to continue to run for a specified period before shut-down.

1. From the main menu, select **CONFIGURATION>OPTIONS**.
2. Click the **Leak Detection** tab.

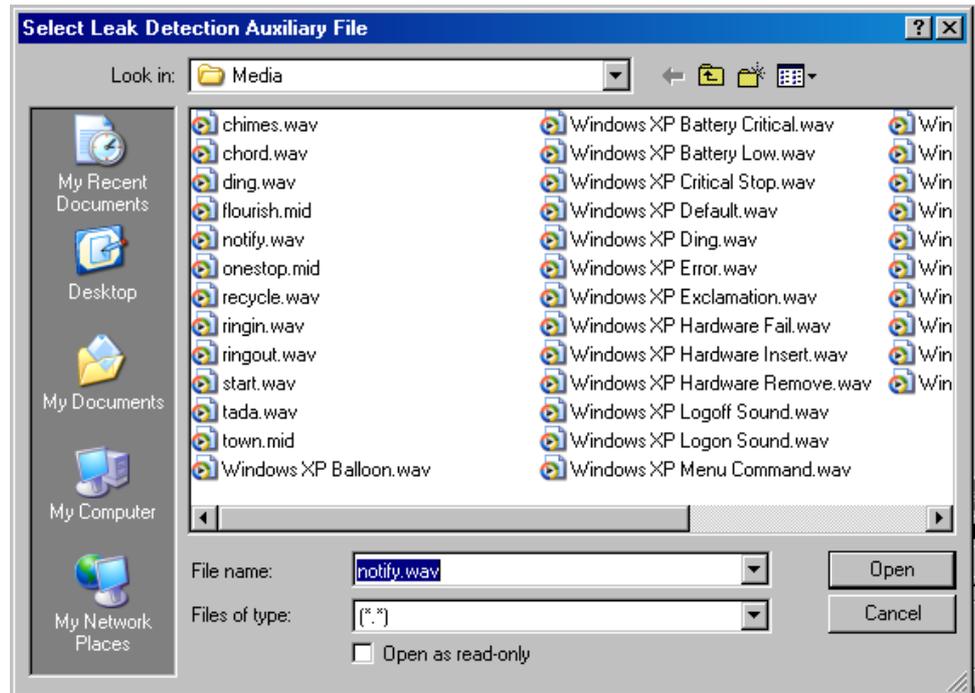


3. Enter a value (0–90 minutes) in the “Stop All Processing Period” box.



4. Click the **BROWSE** button in the Program line to specify the program (e.g. Windows Media Player) to run the alarm file. Select “Run Minimized” to run the program in the background.
5. Check the Launch Program When Leak Is Detected box.
6. Click the **BROWSE** button in the Arguments line.

7. Highlight a file, then click **OPEN** to select the file for the alarm. Click **TEST** to hear the alarm.



8. To set a repeat interval for the alarm, check the "Launch Program Recurringly" box and designate the interval (1–90 minutes) in the "Recurring Period (min)" box.
9. If a control bit has not been assigned to the Leak Sensor, the alarm period and interval cannot be set in the Leak Detection options.

Section 4 QuikChem 8000 system configuration

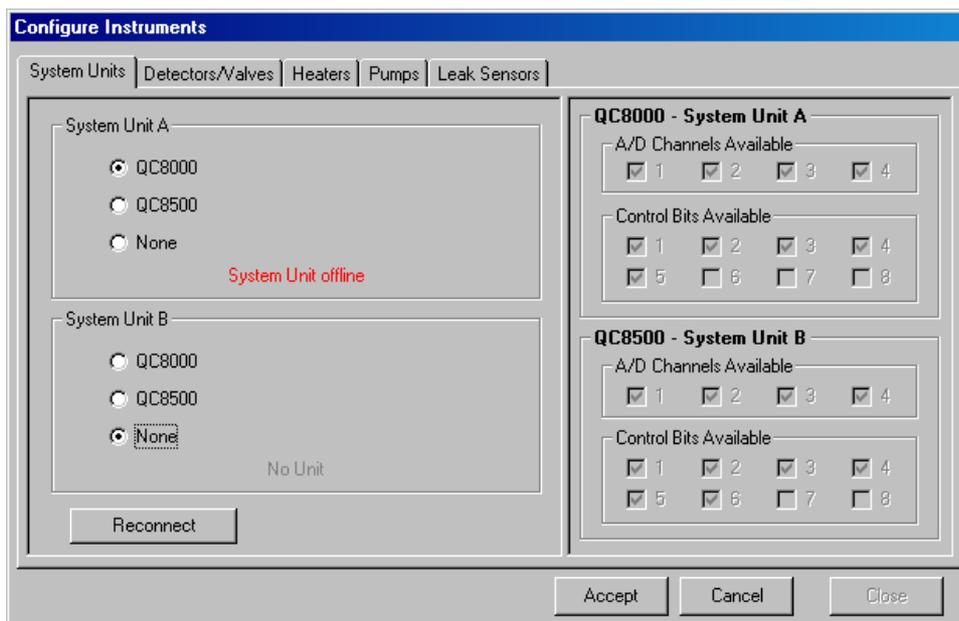
4.1 Configuring the QuikChem 8000

Note: Computers supplied by Lachat Instruments are factory-configured for QuikChem systems. Proceed to [Section 9, Run setup, on page 47](#). For all other computers, configure the system before proceeding with the Run Analysis.

Omnion 3.0 software supports the QuikChem 8000 and the QuikChem 8500 (section [3.1 on page 11](#)) as individual systems. The software can also be configured for using both systems together (section [5.1 on page 23](#)).

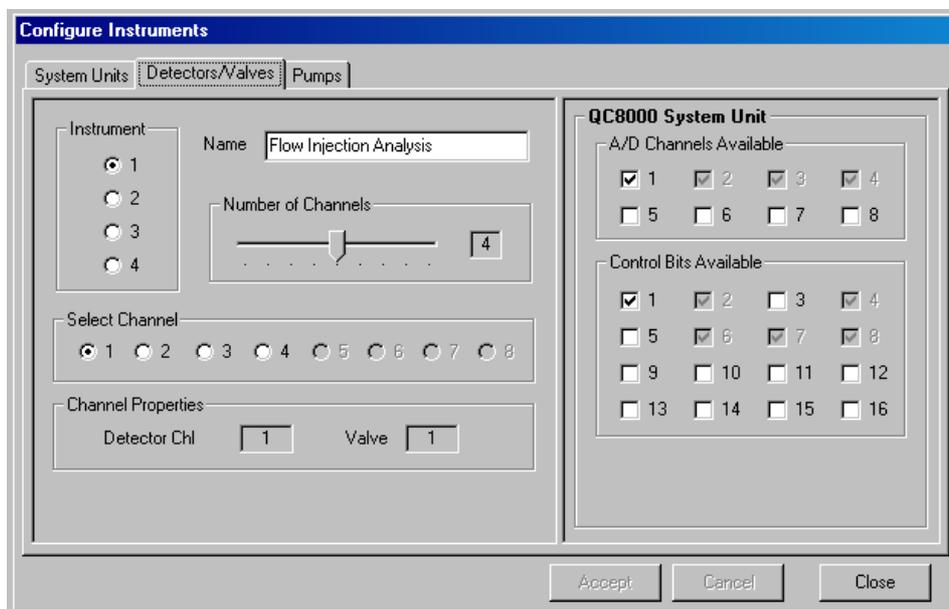
4.1.1 Instrument configuration

1. Start Omnion 3.0 software using the desktop icon or the Windows toolbar.
2. From the main menu, select **CONFIGURATION>INSTRUMENTS**.
3. Click the **System Units** tab. Select QC8000.



Note: An Instrument is a collection of hardware and software resources needed to make a run. Each run has only one instrument associated with it. The default system configuration is set for 4-channel FIA instrument configured as Instrument 1. This default configuration may need to be adjusted to accommodate system specification.

4. Click the **Detectors/Valves** tab.
5. Select Instrument 1, 2, 3 or 4 to configure.
6. Enter a name for the instrument. For example, if the instrument was used to run a two-channel flow injection analysis measurement, a possible name is "Flow Injection Two-channel Instrument".



7. Drag the slider to the desired number of channels. For the 8000 instrument, if one NI board is installed, the maximum number of channels will be 4, and if there are two NI boards installed, the maximum number of channels will be 8.

Note: A Run can have from 1–8 channels. However, if the Run has more channels than its instrument, when Preview of Start Run is selected, a “Run needs more channels than Instrument (Instrument Name) has” message appears, and the Run will stop immediately. In this case, either add more channels to the Instrument Configuration, or delete channels from the Run.

8. Select the Channel number to configure. Each instrument channel can be configured individually.
9. Select the position for the A/D channel and the control bit setting. See [Table 3](#).

Note: If the position is unavailable, verify that these resources are not currently being used with another instrument. Only one channel can use each A/D channel and control bit.

Table 3 Typical Channel Configuration

Channel No	1	2	3	4	5	6	7	8
A/D (Detectors)	1	2	3	4	5	6	7	8
Control Bits ¹ (Valves)	1	2	3	4	9	10	11	12

¹ Control Bits 5 through 8 are used as pump controls.

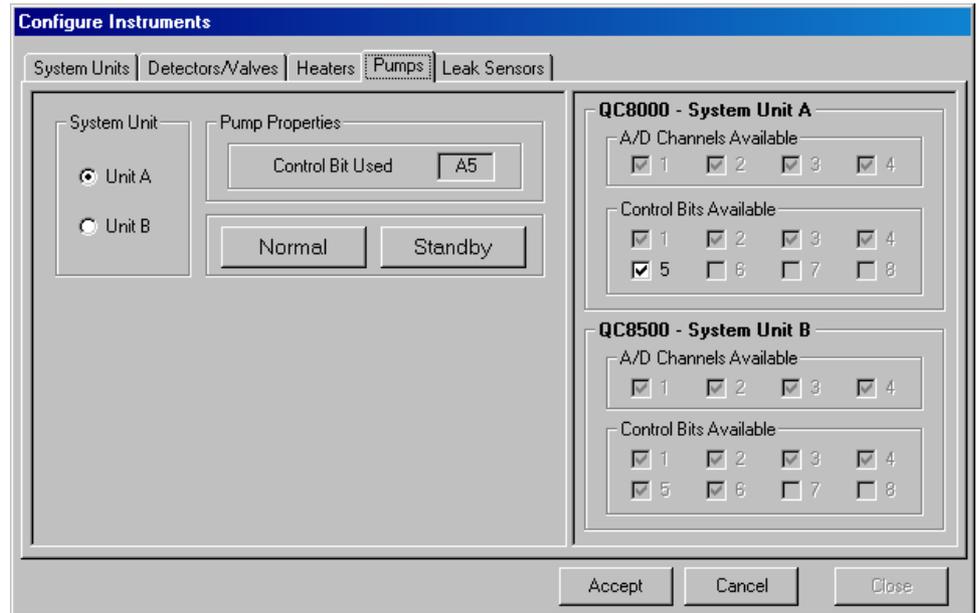
10. Click **ACCEPT** to save changes. Click **CLOSE** to leave the configuration.

Note: Changes cannot be made during a Run. Click **CLOSE** to leave the configuration unchanged.

11. Follow steps 1–9 to add additional instruments to the Configuration.

4.1.2 Pump control

The system pump(s) is configured in the Configure Instruments screen.



1. Click the **Pumps** tab to access the Pump configuration screen.
2. Select System Unit A or B.
3. If necessary, change the speed of the pump to standby or normal speed.
4. Click **ACCEPT**, then click **CLOSE** to exit the pump configuration screen.

Section 5 QuikChem 8500/8000 system configuration

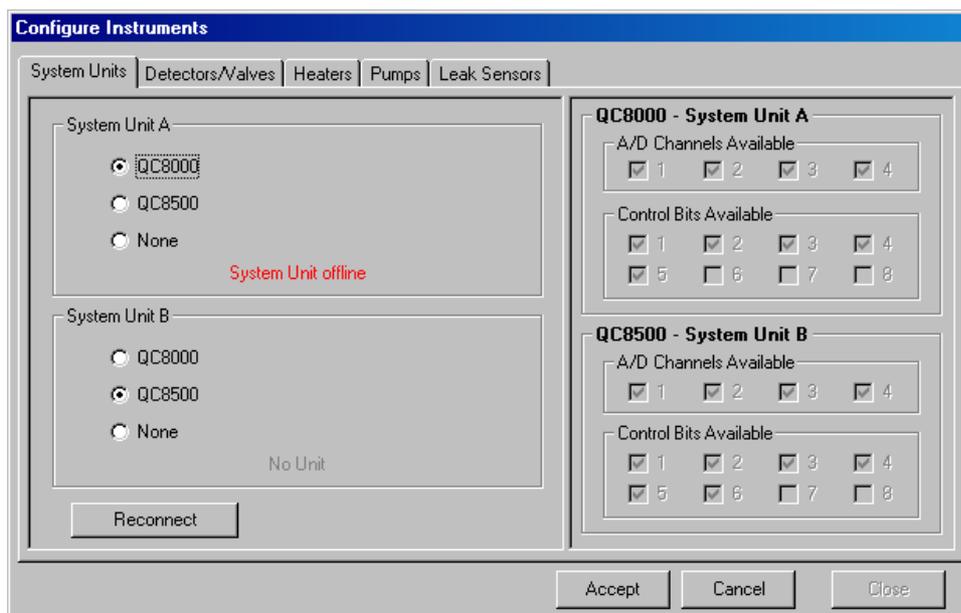
5.1 Configuring QC8500 and QC8000 together

Note: Computers supplied by Lachat Instruments are factory-configured for QuikChem systems. Proceed to [Section 9, Run setup, on page 47](#). For all other computers, configure the system before proceeding with the Run Analysis.

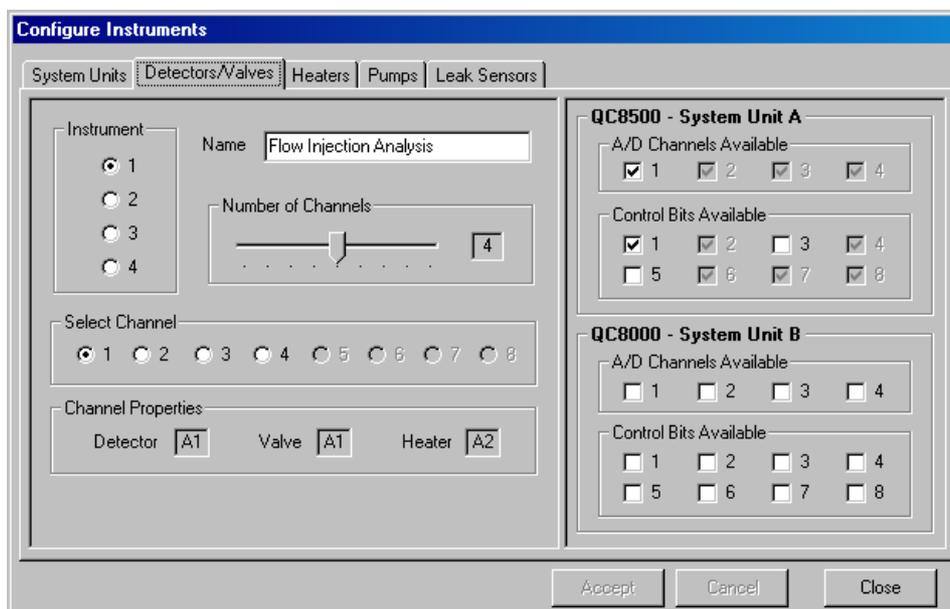
Omnion 3.0 software can be configured for using both the QC8000 and the QC8500 together. The software also supports the QuikChem 8000 (section [4.1 on page 19](#)) and the QuikChem 8500 (section [3.1 on page 11](#)) as individual systems.

5.1.1 Instrument configuration

1. Start Omnion 3.0 software using the desktop icon or the Windows toolbar.
2. From the main menu, select **CONFIGURATION>INSTRUMENTS**.
3. Click the **System Units** tab. Select the system assigned to Device 1 and the system assigned to Device 2.



- Click the **Detectors/Valves** tab. Enter the name of the run.



- Select Instrument 1, 2, 3 or 4 to configure.
- Drag the slider to the desired number of channels.
- Select the Channel number to configure. Each instrument channel can be configured individually.
- Select the position for the A/D channel and the control bit setting.

Note: If the position is unavailable, verify that these resources are not currently being used with another instrument. Only one channel can use each A/D channel and control bit.

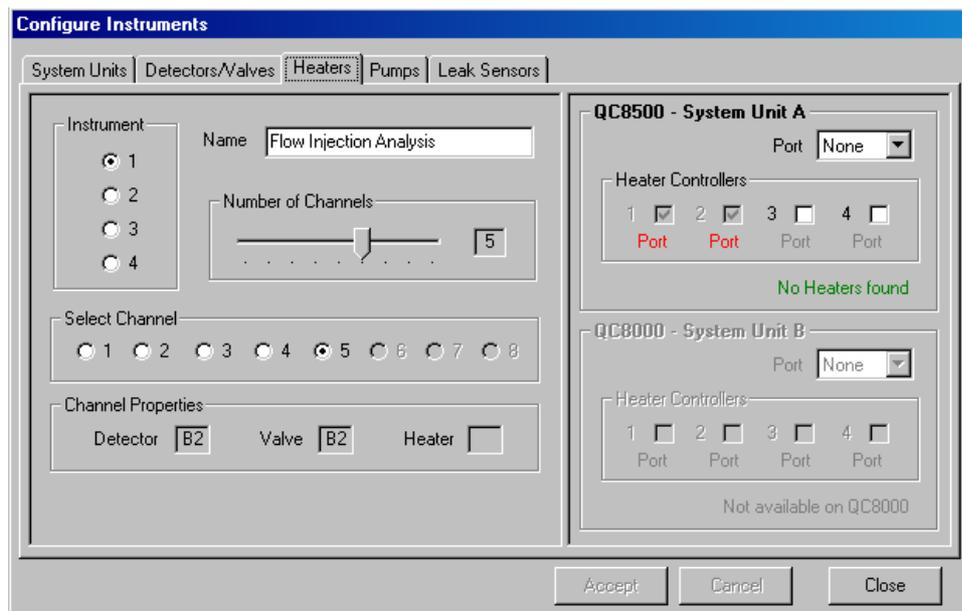
- Click **ACCEPT** to save changes. Click **CLOSE** to leave the configuration screen.

Note: Changes cannot be made during a Run. Click **CANCEL** to leave the configuration unchanged.

Follow steps 5–9 to add additional instruments to the Configuration.

5.1.2 Heater configuration—QC8500 only

1. Click the **Heaters** tab to access the heater configuration screen.



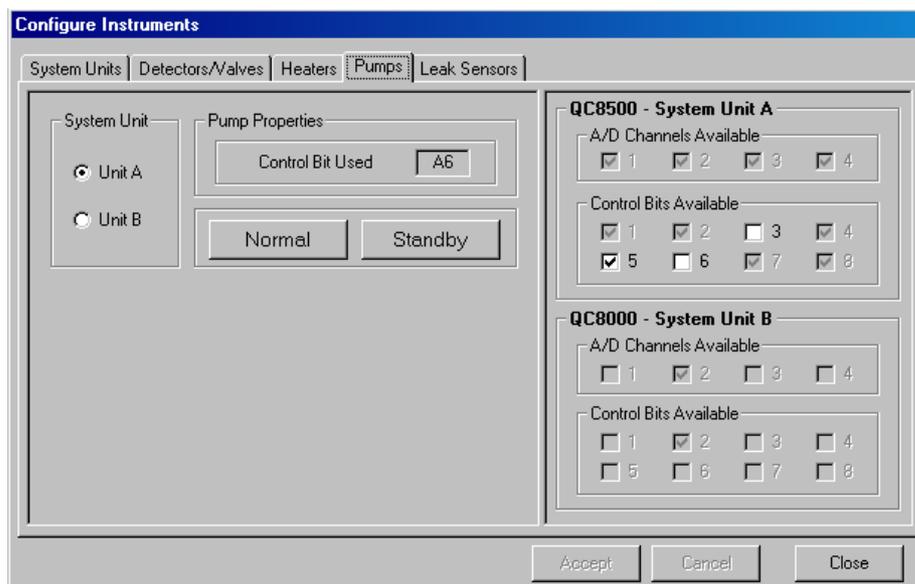
Note: Heater configuration is not available for the QC8000.

2. Select an available port for the QC8500 system unit.
3. Click **ACCEPT**, then click **CLOSE**.

See [Setting the heater options on page 14](#) to set when heater warm-up begins. See [Setting the run properties on page 50](#) to set the temperature for the heater.

5.1.3 Pump control

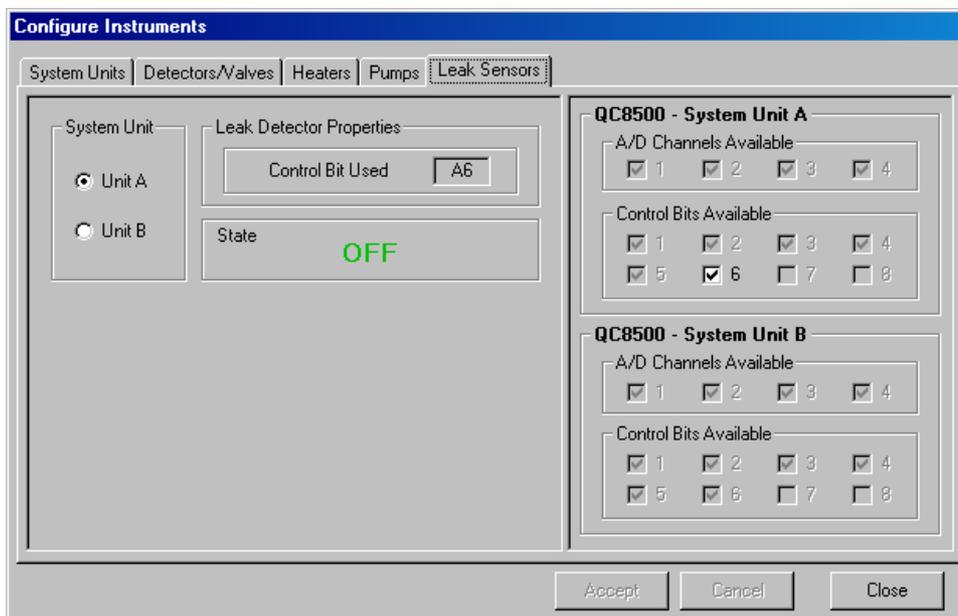
The system pump(s) is configured in the Instrument Configuration screen.



1. Click the **Pump** tab to access the Pump configuration screen.
2. Select System Unit A or B.
3. If necessary, change the speed of the pump to standby or normal speed.
4. Click **ACCEPT**, then click **CLOSE** to exit the pump configuration screen.

5.1.4 Leak sensor status—QC8500 only

1. Click the **Leak Sensors** tab to access the leak sensor configuration screen.



2. Select System Unit A or B. Click **ACCEPT**, then click **CLOSE**. See [Leak sensor status on page 15](#) for alarm settings.

Section 6 Configuring the autosampler

6.1 Autosampler setup

Note: Configuration of autosamplers is the same for the QuikChem 8500 and the QuikChem 8000.

The QuikChem system can support up to four autosamplers or manual samplers. Each of these four autosamplers have a tab where its properties can be configured or defined.

1. From the main menu, select **CONFIGURATION>AUTOSAMPLERS**. The Configure Autosampler window appears.

The screenshot shows the 'Configure Autosampler' dialog box with the following settings:

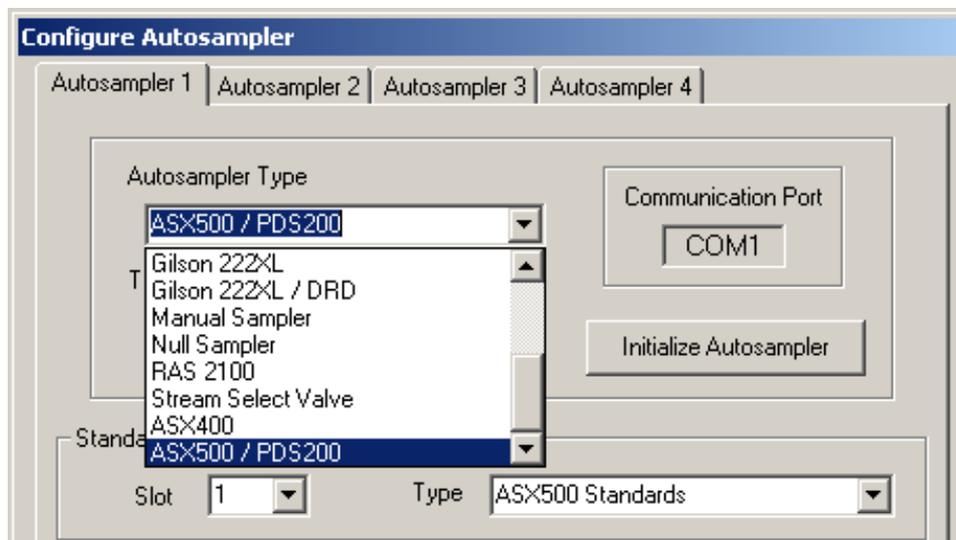
- Autosampler Type: ASX500
- Tray: ASX500
- Communication Port: COM1
- Standards Rack Slot: 1
- Standards Rack Type: ASX500 Standards
- Sample Cup Depth: 120
- Wash Bath Depth: 160

2. Select the appropriate **Autosampler** tab (Autosampler 1–4).

Note: If the system includes an autodilutor, configure the sampler and dilutor together. See [Section 7 on page 31](#).

Configuring the autosampler

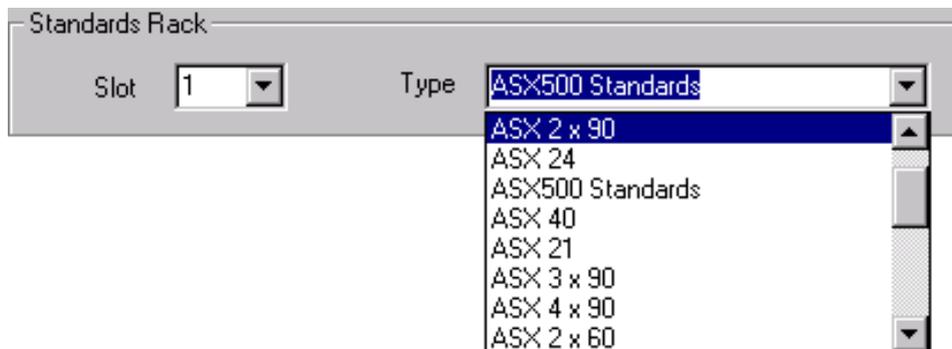
3. Select the type of autosampler with the appropriate option (dilutor) from the drop-down box. If there is no autosampler, select None. In addition to several autosamplers, both systems support a Manual Sampler which will prompt for sampling, and a Null Sampler, which will not prompt (i.e., the Null Sampler runs continuously).



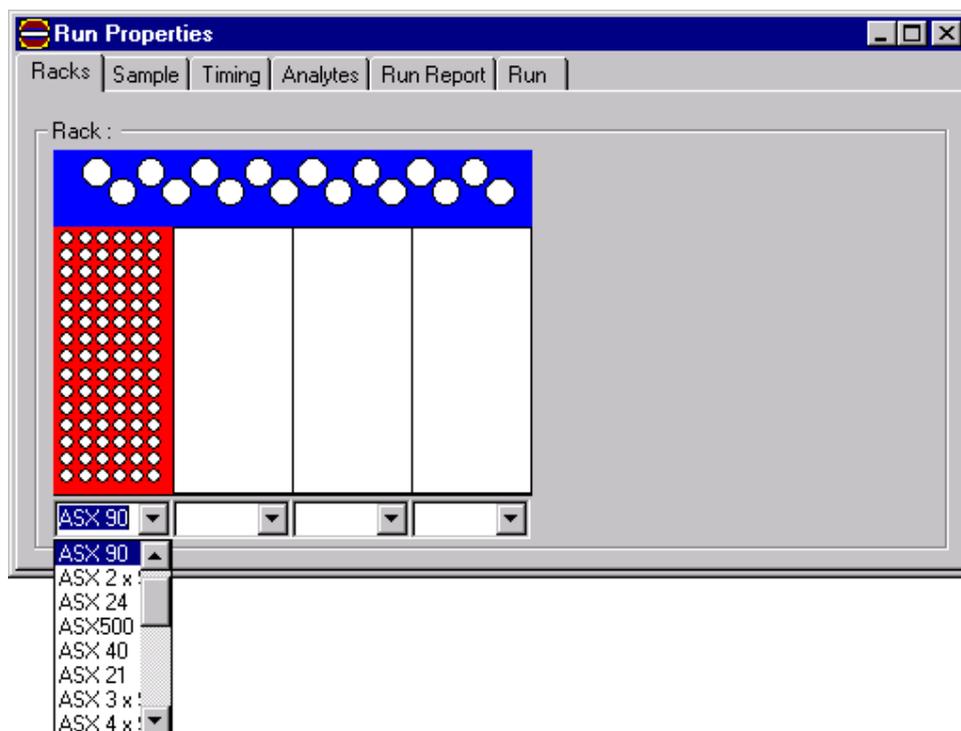
4. Select the desired probe depth (mm) for the sample cups and wash bath. The default settings maximize probe depth. Probe depth can be reduced by decreasing sample cup depth or wash bath depth.

Note: Dilutor rack settings are only available if the system has an autodilutor.

5. Once the Autosampler Type is selected, the Tray, Standards and Dilution Rack settings are filled with the typical or default values. If necessary, change the rack types for the Standards or Dilution racks.
 - a. To select a rack type, select the Type drop-down menu and select the appropriate rack type.



- b. To view the standards rack, click the **Racks** tab in the Run Properties window.



Note: Only the Standards and Dilution Racks are configured in the Configure Autosampler section. Each sampler can have only one standards rack. The default setting is labeled as the Standards Rack under the Type drop-down menu.

Note: For all autosamplers except the Gilson 222, Slot 1 should be selected for the Standards Rack and the last available tray slot is automatically used for the Dilution Rack. For the Gilson 222, Slot 5 should be selected for the standards rack and Slot 4 for the dilution rack.

6. If necessary, set the Autodilution Factors.

The Low, Medium and High Auto Dilution Factors show the default settings that may be used when a dilution is triggered by an over range sample. If a peak is off-scale (% of high standard), or larger than the highest calibration standard, the sample will be rerun at the end of the tray using the appropriate dilution factor selected by the system. The system will automatically select the low, medium or high factor based on the size of the peak.

Note: For optimal triggered dilutions, these settings should not be adjusted.

7. If necessary, change the COM port. Click the **CHANGE PORTS** button. The Autosampler/Dilutor COM port box will appear. Click the drop-down box and select either COM 1 or 2. Click **OK** and **CLOSE** to exit.

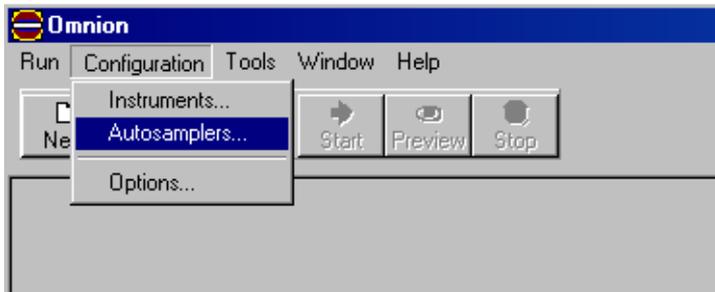
Configuring the autosampler

8. Depending on the type of autosampler, a prompt may be displayed to enter a COM port setting for both the Autosampler and Dilutor. Select the appropriate COM ports for each component. Click **OK** after making the appropriate solution, then select **CLOSE** to exit the Autosampler Configuration screen.
9. Click **APPLY** to set the changes.

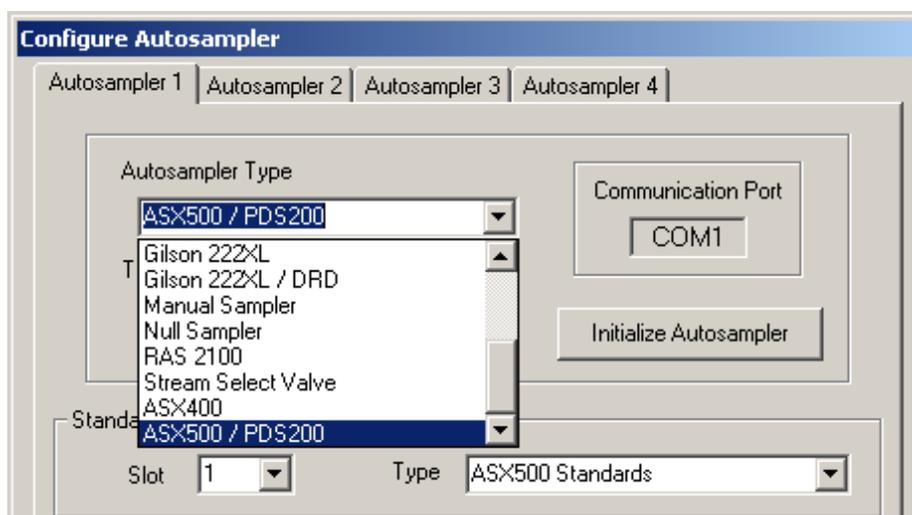
Section 7 Configuring the dilutor

7.1 Configuring the PDS200 dilutor

1. In the Omnion software, select Autosamplers... from the Configuration menu.

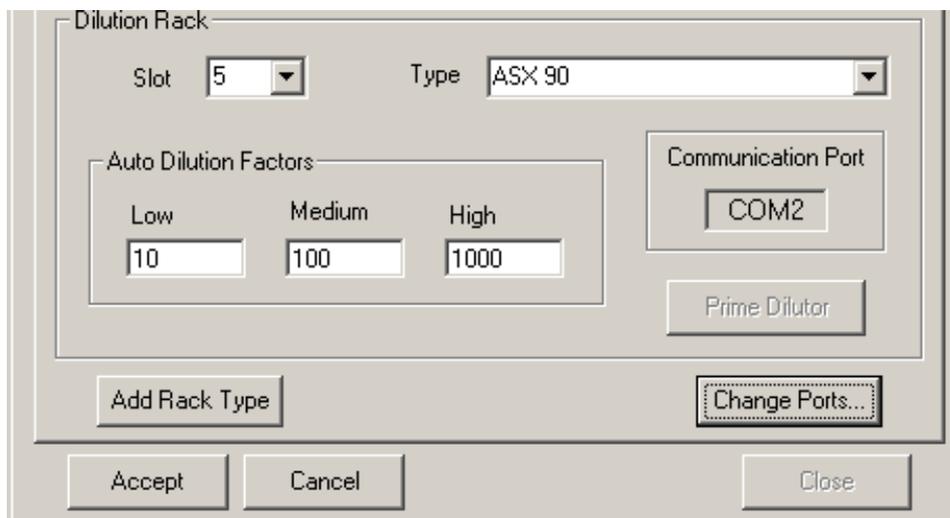


2. In the Configure Autosampler dialog box, select "ASX500/PDS200" from the Autosampler Type menu.

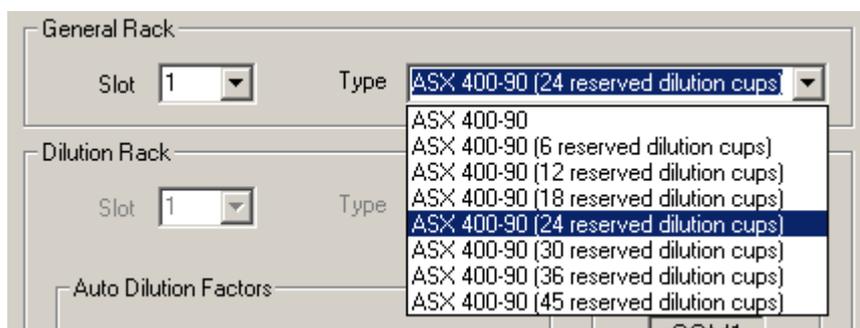


3. Select General Rack.

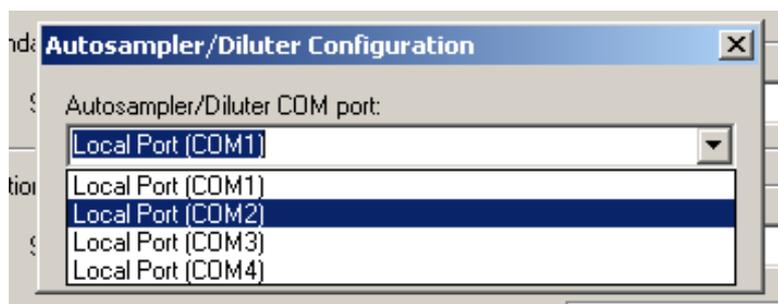
Note: For the ASX-410, the number of dilution cups needs to be selected. The cups are placed at the end of the 90-position rack. If the **Racks** tab is selected in Run Properties, the dilution cups for the ASX-410 will be shaded in red.



4. To designate a different COM port for the autosampler, click **CHANGE PORTS** and go to step 5. (COM1 is the default setting.)



5. Select the new COM port from the Autosampler/Diluter COM port list and click **OK**.



Note: Refer to [Table 5 on page 49](#) for more information on sample dilutions.

6. Click **ACCEPT** to confirm the communication port and autosampler/diluter combination.

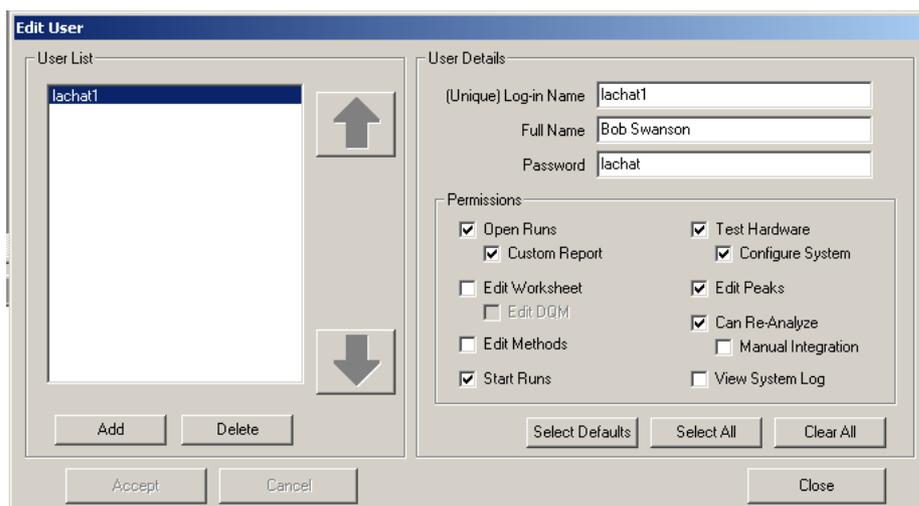
The screenshot shows a software dialog box titled "Dilution Rack". At the top, there are two dropdown menus: "Slot" with the value "5" and "Type" with the value "ASX 90". Below these is a section titled "Auto Dilution Factors" containing three input fields: "Low" with the value "10", "Medium" with the value "100", and "High" with the value "1000". To the right of this section is a "Communication Port" dropdown menu showing "COM2". Below the "Communication Port" menu is a "Prime Dilutor" button. At the bottom of the dialog, there are three buttons: "Add Rack Type", "Change Ports..." (which is highlighted with a dashed border), and "Accept". At the very bottom of the window, there are three buttons: "Accept", "Cancel", and "Close".

Section 8 Configuring general Omnion options

8.1 Security

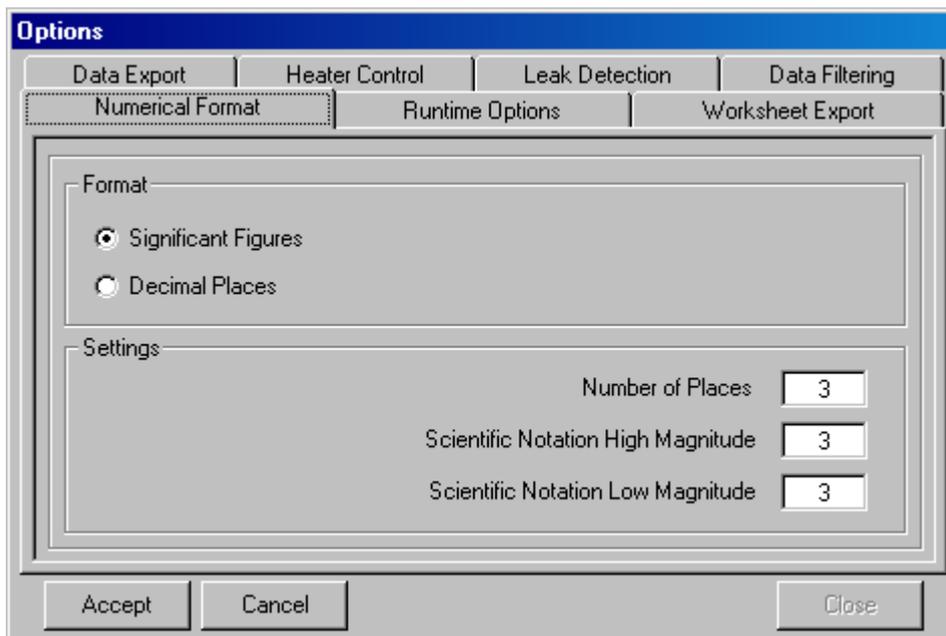


1. From the Main Menu, select **CONFIGURATION>ENABLE SECURITY**. Enter the user name and password. The user name for the administrator is Admin (case sensitive). The password for the administrator can be obtained by calling Lachat Technical Support. Obtain the administrator password by calling Lachat Technical Support.
2. Once security has been enabled, another menu option appears on the top line. Within this menu passwords can be changed and different users can be assigned by the administrator.
3. When the **User** tab is selected, rights and privileges can be assigned for different users.



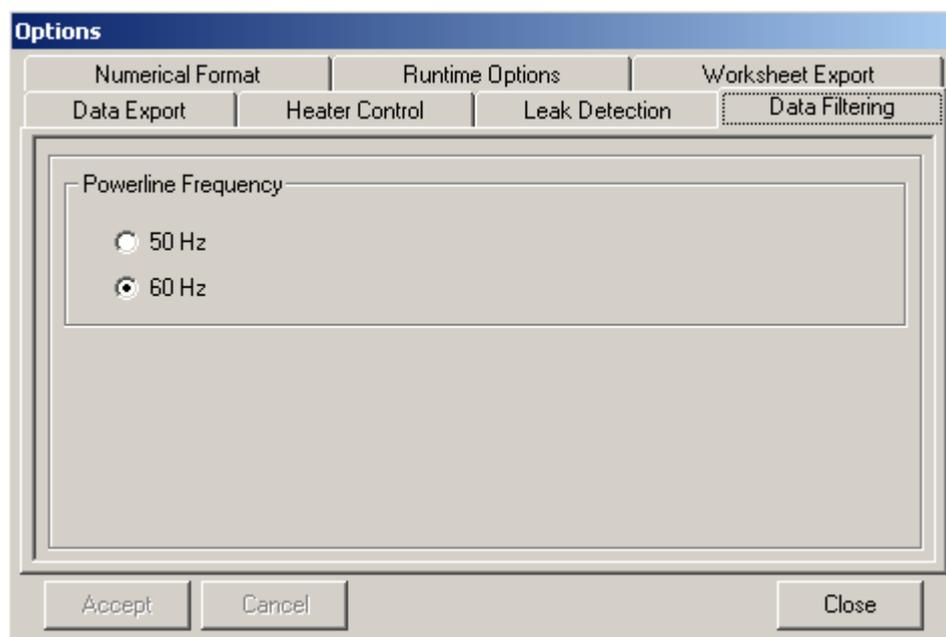
8.2 Changing the electrical power frequency

1. From the main menu, select **CONFIGURATION>OPTIONS**. The Options window will appear.



Note: For systems in the United States, select 60 Hz. In most EU countries, the powerline frequency is 50 Hz. For all other countries, consult with an electrician to determine local powerline frequency.

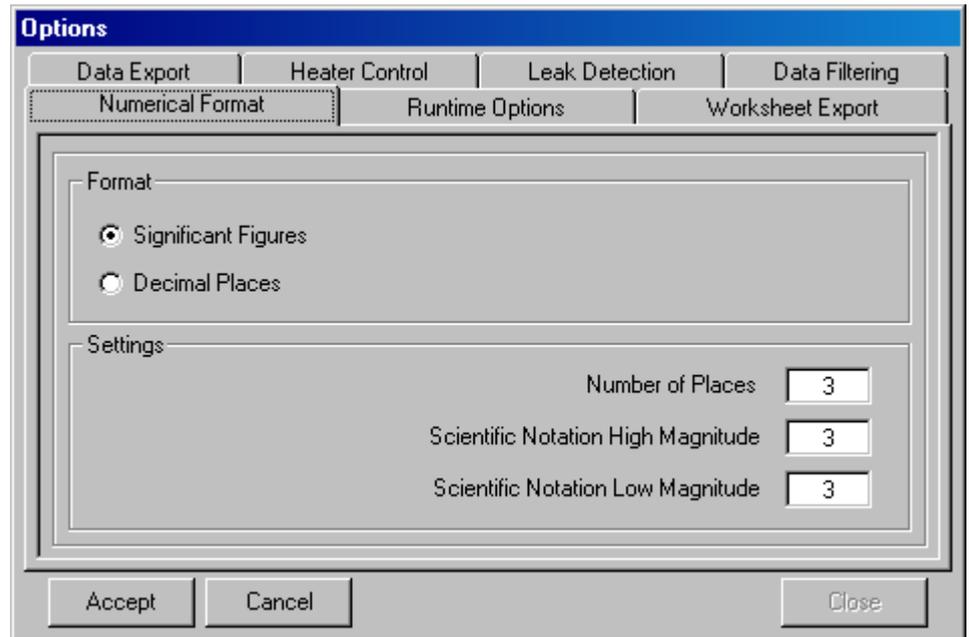
2. Click the **Data Filtering** tab. Select the electrical frequency appropriate for the location of the instrument. Click **ACCEPT**, then **CLOSE**.



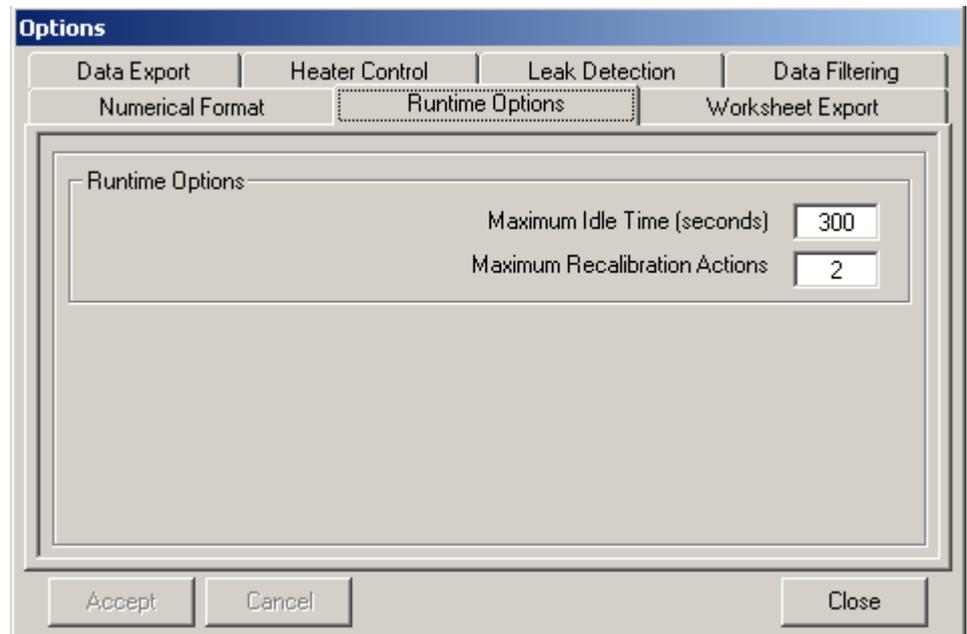
8.3 Setting runtime options

Runtime options control:

- the maximum idle time (in seconds) before the run stops automatically
 - the maximum number of recalibration actions per run
1. From the main menu, select **CONFIGURATION>OPTIONS**. The Options window will appear.



2. Click the **Runtime Options** tab. Enter the value for maximum idle time and maximum recalibration actions. Press **ACCEPT** and **CLOSE**

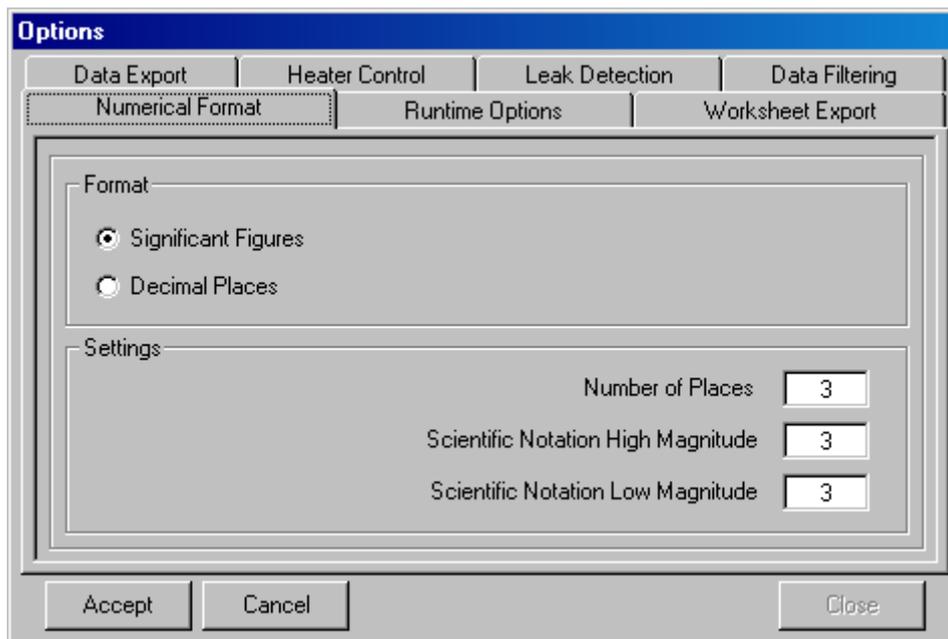


8.4 Printing and exporting worksheets

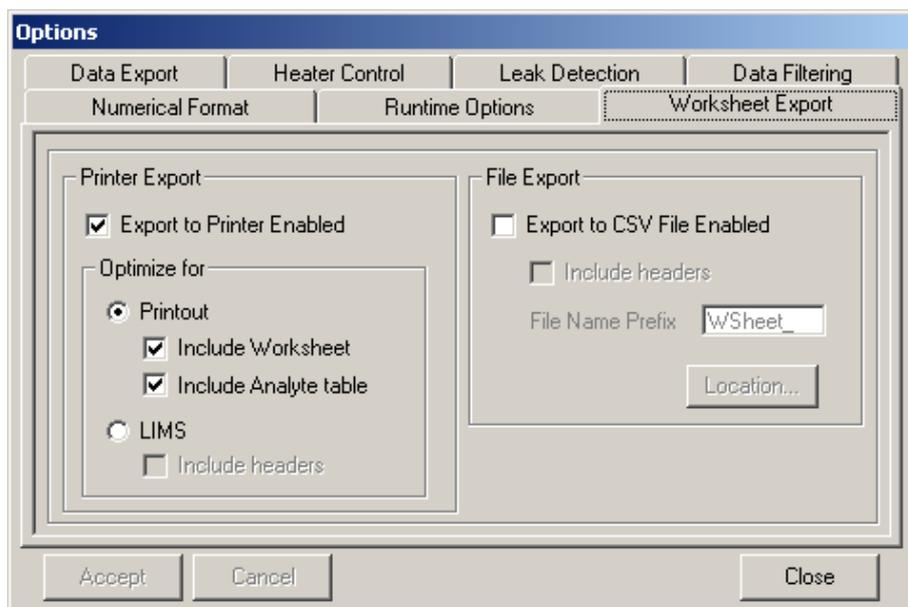
After entering sample data into the Run Worksheet (Section 9 on page 47) the worksheet can be exported to a printer or a CSV file.

8.4.1 Exporting a run worksheet to the printer

1. From the main menu, select **CONFIGURATION>OPTIONS**. The Options window will appear.



2. Click the **Worksheet Export** tab. Set the printer setting as shown below. Press **ACCEPT** and **CLOSE**.



3. From the main menu select **RUN>EXPORT WORKSHEET DATA** to print the data.

There are 3 fields of information in the printout. The first is a header box that always appears. The middle field of the printout is the run worksheet information. This appears in the printout if the Include Worksheet box is checked. The last field of the printout is an analyte table and gives the known concentration of the calibration standards. It appears if the Include Analyte table box is checked.

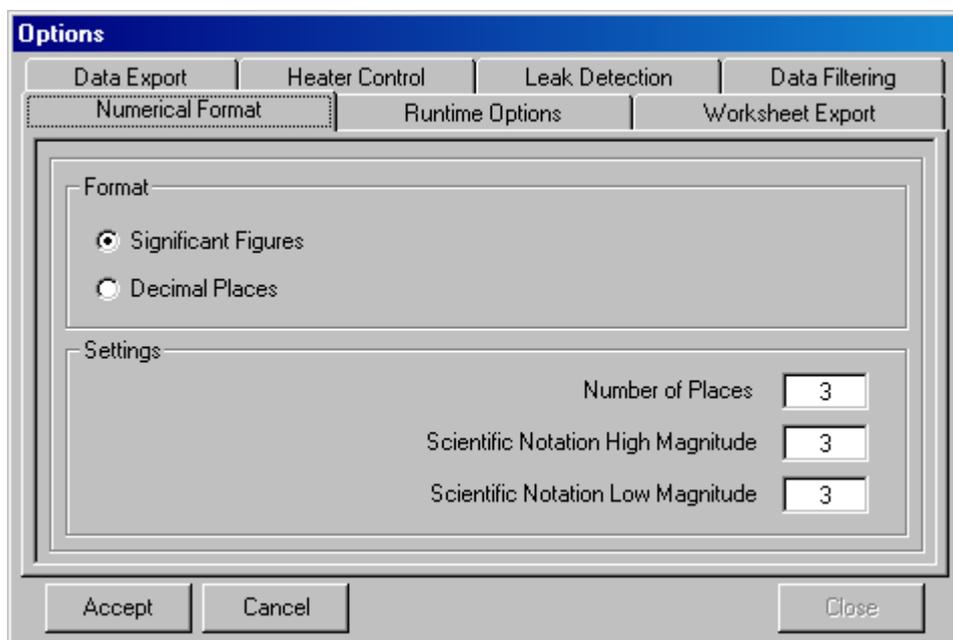
8.4.1.1 Using the LIMS option

The **Worksheet Export** tab has a LIMS (Laboratory Information Management System) option. With the LIMS option selected, worksheet information will be sent to the default printer in CSV format. When printing the worksheet, select one optimized option. The other option will automatically be deselected.

8.4.2 Exporting a run worksheet to a CSV file

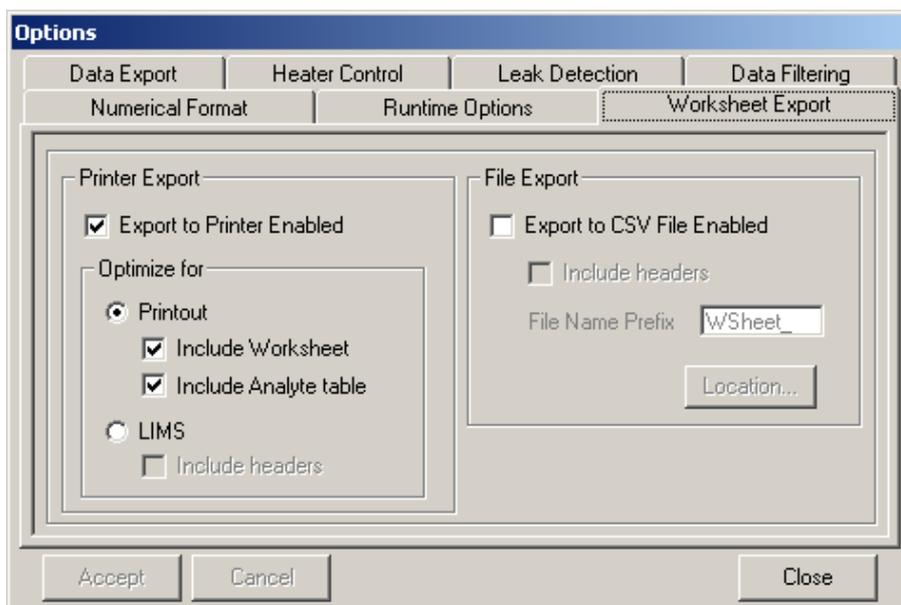
Omnion 3.0 also allows the export of the Run Worksheet to a CSV file. The CSV files will be comma separated. This allows programs such as MS Excel to place the various items exported into separate columns.

1. From the main menu select **CONFIGURATION>OPTIONS**. The Options window will appear.

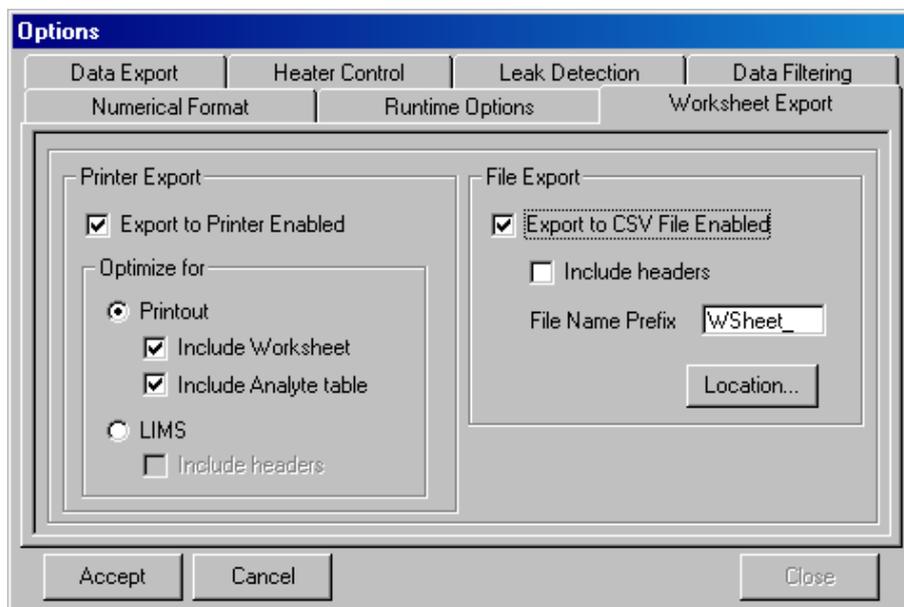


Configuring general Omnion options

- Click the **Worksheet Export** tab. Deselect the Export to Printer Enabled check box to disable the print export function.



- Check the Export to CSV File Enabled check box.



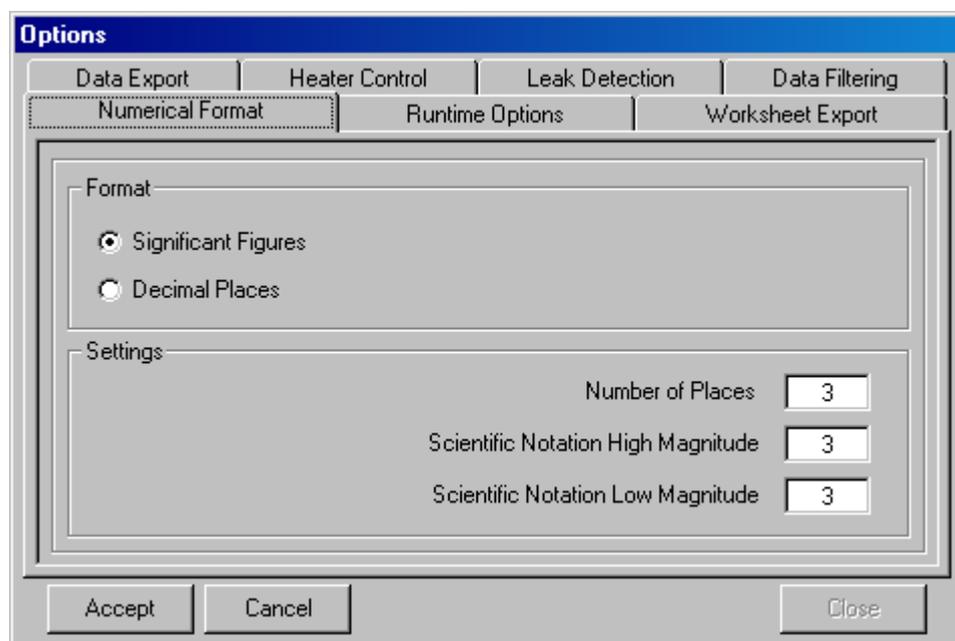
- Check the Include Headers check box to include the headers in the CSV file.
- During the export, a file will be created using the name of the exported run file. Additional text can automatically be added to the beginning of the file name using the File Name Prefix field. The default prefix is WSheet_.
- Click the **LOCATION** button to select where to place the exported file.
- Press **ACCEPT** and **CLOSE**.
- From the main menu select **RUN>EXPORT WORKSHEET DATA** to export the data to the file.

8.5 Exporting data

The data generated while running the Omnion 3.0 software can be exported to a file or a printer. Many users export data to a file so they have the option of working with the data in a spreadsheet program such as MS Excel or importing the data into a LIMS. The CSV files will be comma separated. This allows programs such as MS Excel to place the various exported items into separate columns. Additionally, many users print data so that a hard copy can be kept on file. Data can be exported in a manner similar to exporting the run worksheet. It can be exported to a printer or exported and printed from custom reports.

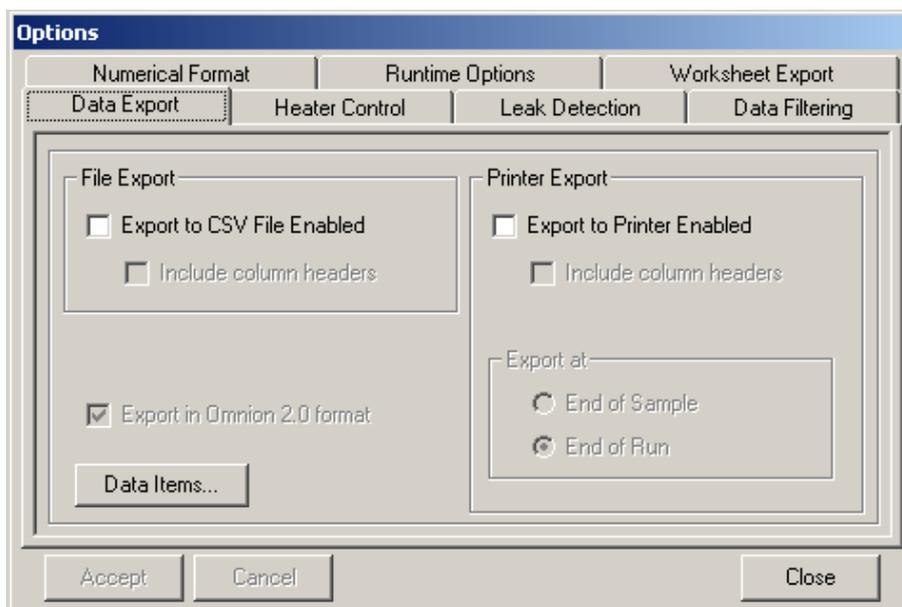
8.5.1 Exporting data to a file

1. From the main menu, select **CONFIGURATION>OPTIONS**. The Options window will appear.

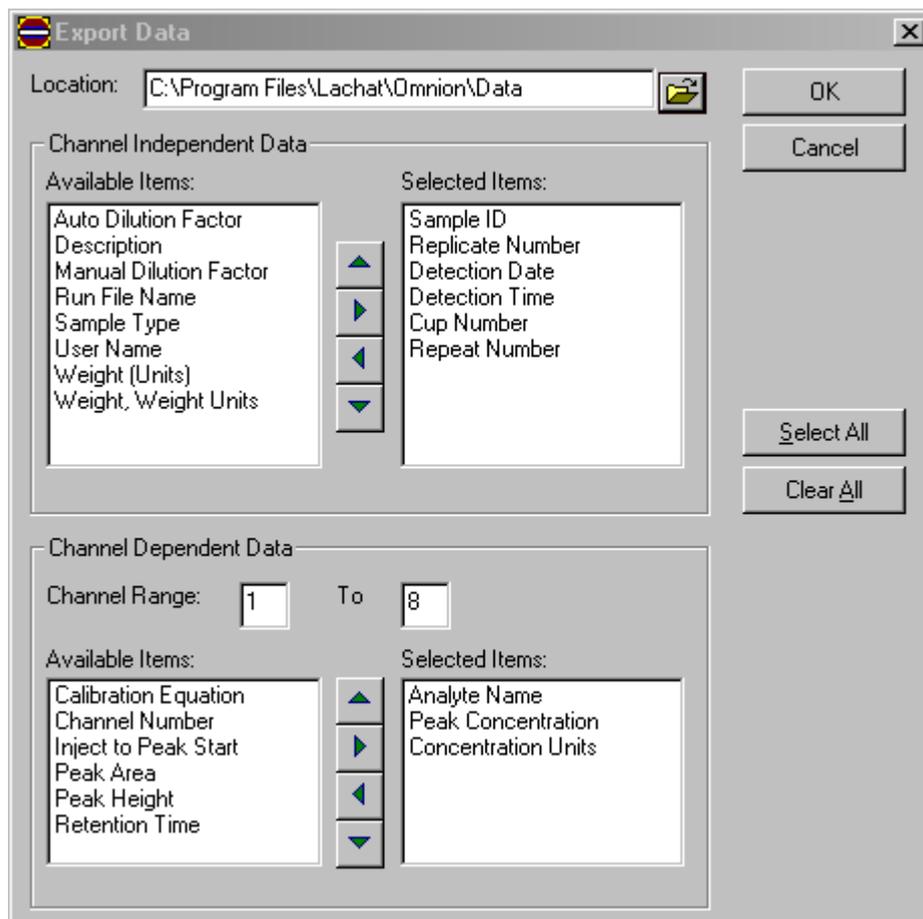


Configuring general Omnion options

- Click the **Data Export** tab. Within this window data can be exported to a CSV file or the printer.



- Click the **DATA ITEMS** button. The Export Data window will appear.





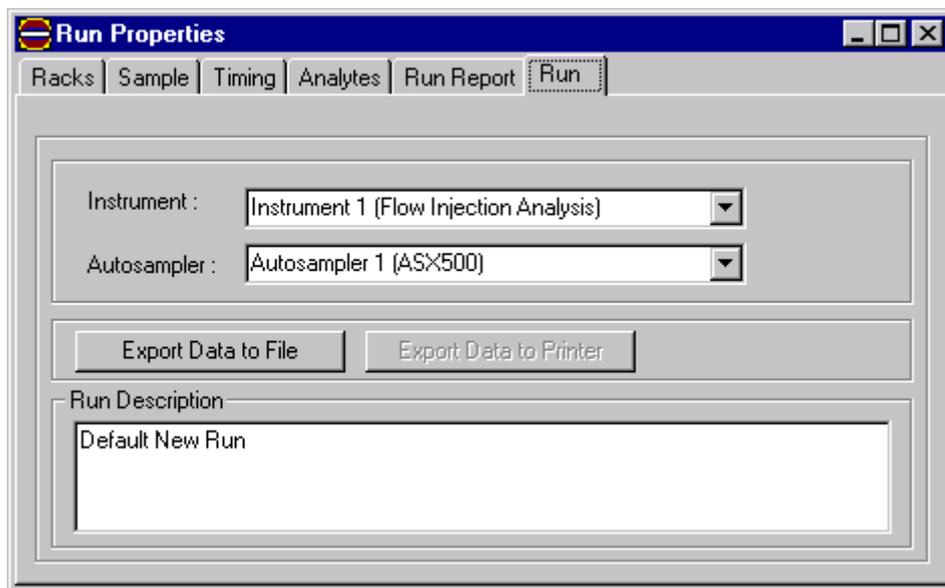
4. Click the **BROWSE** button to select the Location of the data to be exported.

The items that can be exported are categorized as either Channel Independent or Channel Dependent. Each of these categories shows two fields, one for Available Items and the other for Selected Items. The Selected Items will be exported.

5. Select the items to export using the arrow keys. The right arrow key will move an item from the Available Items list to the Selected Items list. The left arrow will move an item from the Selected Items list to the Available Items list. Click the **SELECT ALL** button to select all of the items at one time. Click **CLEAR ALL** to clear the selected items list.
6. Organize the items in the Selected Items list. The order items appear in the Selected Items list will be the same order in which they will appear in the exported data. Use the **UP** and **DOWN** arrow keys to arrange the items.
7. Click **OK** to return to the **Data Export** tab on the Options window.
8. Under File Export, select the Export to CSV File Enabled check box. If necessary, select the Include Column Headers check box. Enable or Disable Export Data in Omnion 2.0 format, depending on user preference.

***Note:** Disabling Export in Omnion 2.0 format will export data with an additional row in the spreadsheet per sample for each analyte that is being reported. When the data is exported from a run that contains data for two analytes, all the information for one of the analytes will appear in columns and the information for the second analyte will appear in columns on the next row of the worksheet. If Export Data in Omnion 2.0 is selected, the data will be exported with the additional analytes appearing in additional columns and only one row of data per sample.*

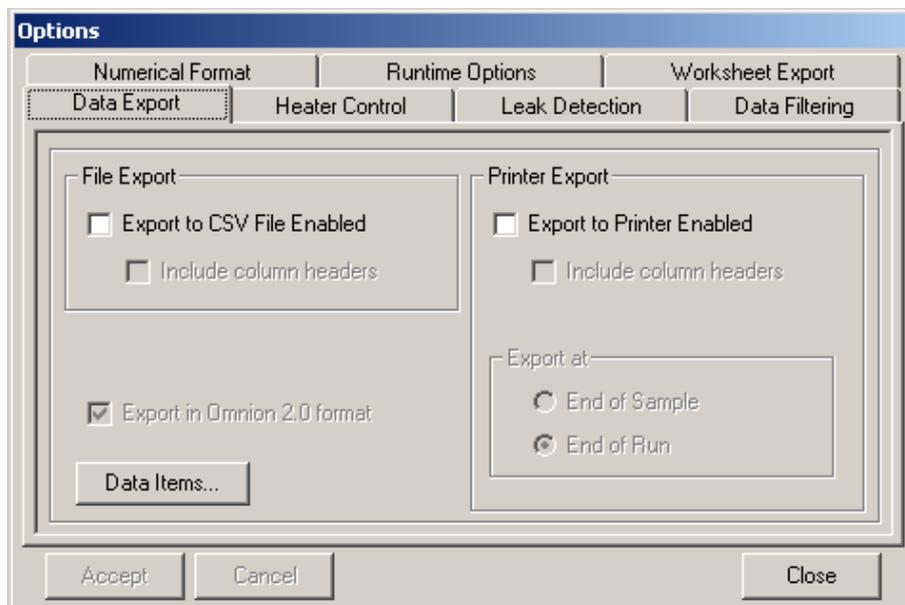
9. Click **ACCEPT** and **CLOSE**.
10. Click the **EXPORT DATA TO FILE** button in the **Run** tab of the Run Properties window to export the data.



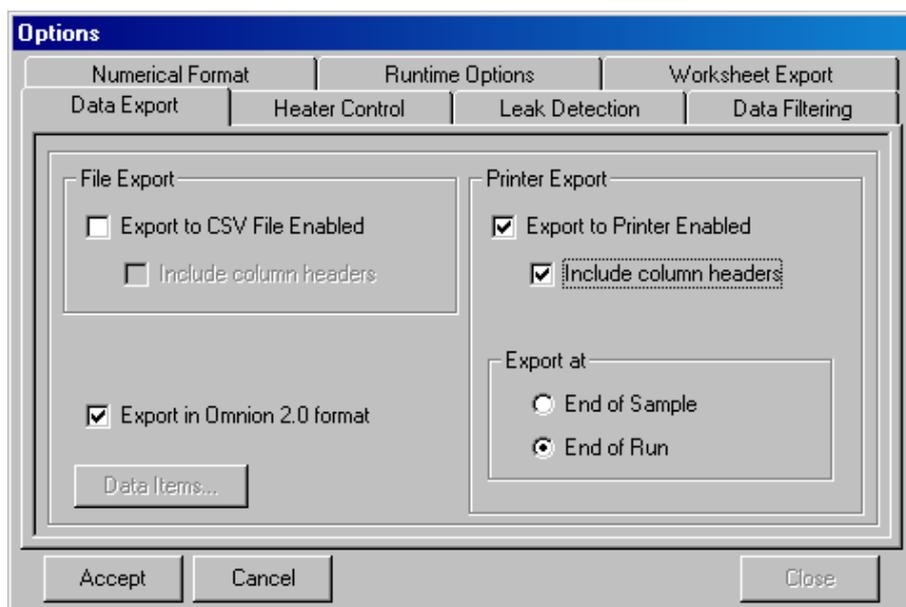
8.5.2 Exporting data to a printer

Note: Omnion 3.0 will use the Windows default printer. The data exported to the printer will be the same Data Items defined in the **Data Export** tab of the options window.

1. From the main menu, select **CONFIGURATION>OPTIONS**. The Options menu will appear. Click the **Data Export** tab.



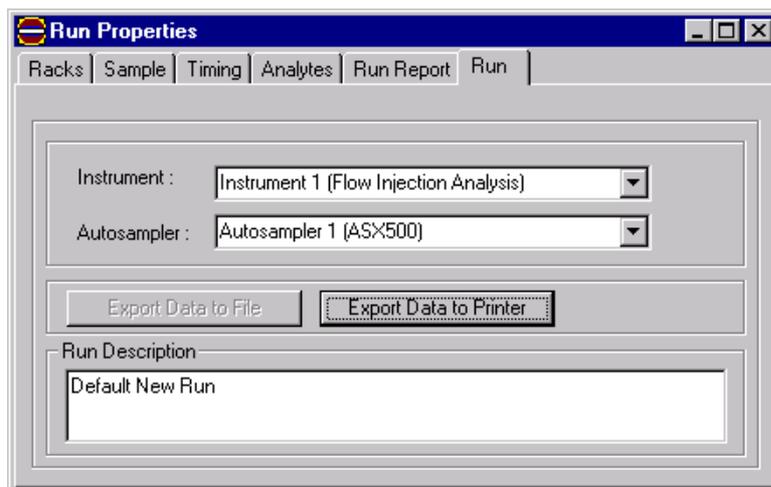
- Under File Export, select the Export to Printer Enabled check box. If necessary, select the Include Column Headers check box.



- Select End of Sample or End of Run before starting a run to print export automatically at the End of the Sample or Run.
- Enable or Disable Export in Omnion 2.0 format, depending on preference.

Note: Disabling Export in Omnion 2.0 format will export data with an additional row in the spreadsheet per sample for each analyte that is being reported. When the data is exported from a run that contains data for two analytes, all the information for one of the analytes will appear in columns and the information for the second analyte will appear in columns on the next row of the worksheet. If Export Data in Omnion 2.0 is enabled, the data will be exported with the additional analytes appearing in additional columns and only one row of data per sample.

- Click **ACCEPT** and **CLOSE**.
- Click the **EXPORT DATA TO PRINTER** button in the **Run** tab of the Run Properties window to print the data.

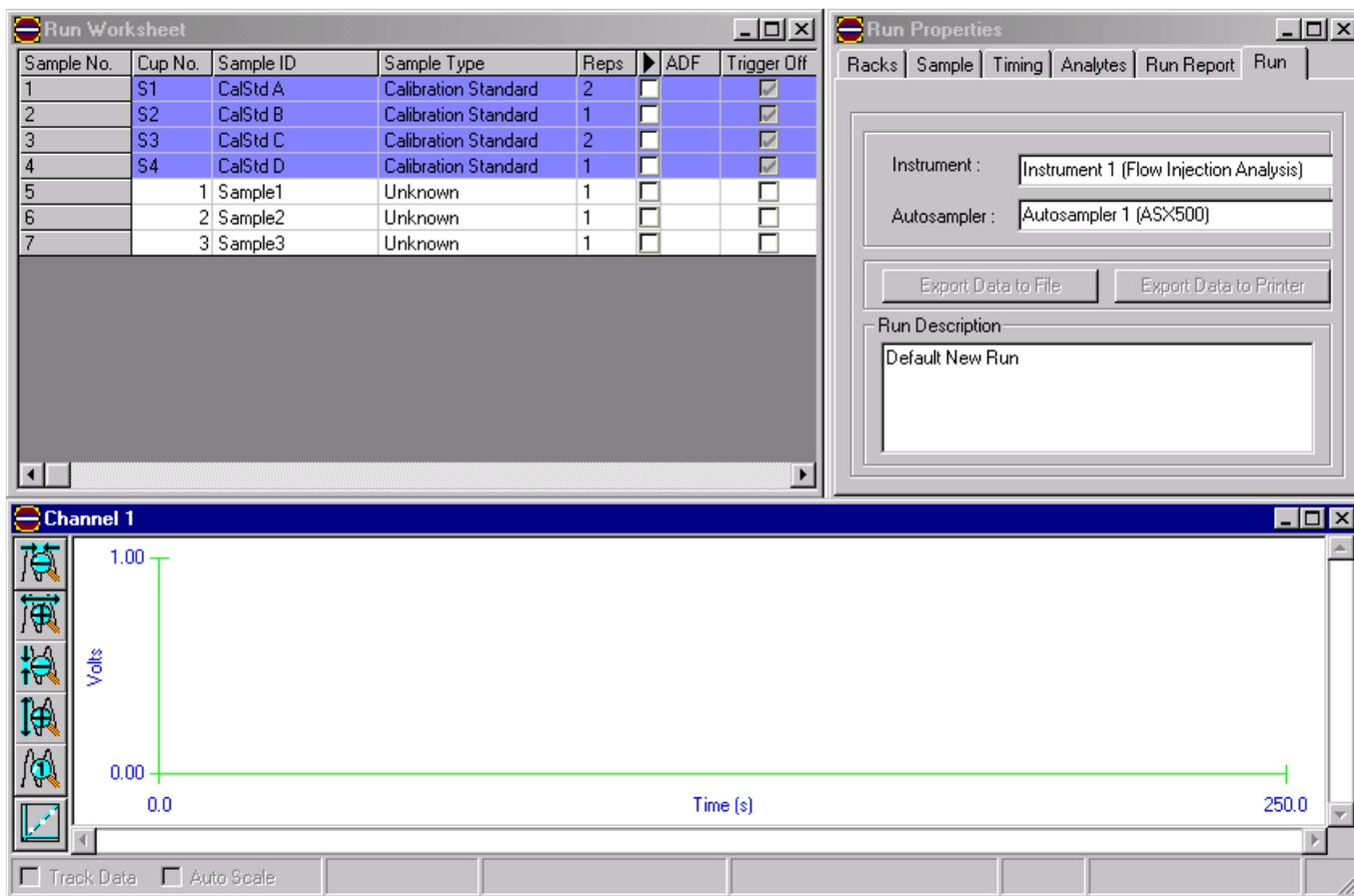


Section 9 Run setup

9.1 Creating a new run and editing the run worksheet

The Run is a self-contained package with everything needed to run samples, acquire data and report data in one place. A Run is saved in an *.omn file. The Run worksheet is the spreadsheet into which all information on the samples is entered. Each row of the Run worksheet is a sample, with its own properties unique to that sample. For daily routine operation, the Run Worksheet may be the only part of the Run that needs to be used.

1. Click the **NEW** button. This will open the Default New Run. Three windows will appear on the screen: the Run Worksheet, the Run Properties and one Channel Data Display.



2. Select a row number from the Sample No. column of the Run Worksheet. The row should be highlighted dark blue.
3. Right-click the row in the Sample No. column to select the editing functions. Refer to [Table 4](#) for Editing functions.
4. After the columns have been setup, enter the information for the appropriate columns in the Run Worksheet by clicking in the field. [Table 5](#) describes all the column features.

Table 4 Editing row functions

Function	Edit instructions
Cut	To delete rows, click and drag along the selected rows, then right-click and select Cut or Delete. Cut will copy the selected rows first, then delete them. Delete immediately deletes the whole selection without copying.
Delete	
Copy & Paste	<p>Contents and rows can be copied and pasted without inserting or deleting new rows. Click a single row, or click and drag along the row to copy information from. In the same Run or another Run, select the same number of rows to paste. The copied information will be pasted into the spreadsheet over existing information. If the same number of rows to paste to are not selected, an error message will be displayed to prevent accidental deletion of row information.</p> <p>When pasting within the same Run, all sample properties, including the properties seen in the Sample tab for that sample, are pasted. When pasting to another Run, only the sample properties that appear in the Run Worksheet and Prep Properties are pasted. This is because the other Run may have different Analyte properties.</p>
Insert	To insert a row or rows before or above a row, click the row to select it, right-click, then click Insert Row or Insert Many. For Insert Many, enter the number of rows to insert and press OK .
Insert Many	
Insert Cut/Copied Rows	To move rows, first Cut them, then click below the row where the new row will be placed. Right-click and select Insert Cut/Copied Rows.
Append Row	To add new rows to the end of the spreadsheet, select any row, then right-click to get the edit menu. Click the Append Row, to add one row or on Append Many, to add more than one row.
Append Many	
Columns	<p>Auto Number Cups: To automatically renumber Cup numbers (No.) in the Samples racks sequentially, click and drag on the rows in the spreadsheet in which the Cup number (No.) sequence should appear. Then right-click and click 'Columns', 'Auto Number Cups'. To renumber all Samples rack Cup Nos. in the Run Worksheet, click the 'Cup No.' header, then right-click, then click 'Auto Number Cups'.</p> <p>All Samples rack Cup Nos., those not in the Standards rack (S1, S2,...), will be renumbered sequentially, incrementing by 1, starting with the first non-Standards rack Cup No. of the selection. If a user-defined DQM Set is included in the selection, its Cup Nos. will not be renumbered because a DQM Set's rows are locked from editing. The Standards rack Cup Nos. (S1, S2,...) are also not renumbered. This allows for a constant arrangement of Calibration Standards, Check Standards and other standards in the Standards Rack, with the ability to renumber the Unknowns in the Samples rack.</p>
	<p>Set Selected Reps: Sets the default number of Replicates. (Reps) is Reps = 1, or run once. Sometimes a series of samples needs to be run in duplicate (Reps = 2), or the same number of Reps. To set all the Reps in a series of selected samples to the same number, click and drag on the Sample Nos. or rows to make the selection, then right-click 'Columns', 'Set Selected Reps'. Enter the number of Reps, then click OK. If a user-defined DQM Set is included in the selection, its Reps will not be changed because a DQM Set's rows are locked from editing.</p> <p>To set all Reps in the Run Worksheet to the same number, click the Sample No. header, then right-click 'Columns', 'Set Selected Reps'. Enter the number of Reps, then click OK.</p>
	<p>Auto Sample ID: To automatically assign Sample IDs to a selection of sequential samples, click and drag on the rows in the spreadsheet in which the Auto Sample ID sequence should appear. Then right-click and click 'Columns', 'Auto Sample ID'. To apply Auto Sample IDs to all Samples in the Run Worksheet, click the 'Sample ID' header, then right-click, then click 'Auto Sample ID'. If a user-defined DQM Set is included in the selection, its Sample IDs will not be changed because a DQM Set's rows are locked from editing.</p>
	<p>Restore Default Column Widths: Click and drag on the right edge of the column header to adjust the column width. The column widths are saved on Save or Save As. To restore the default column widths and to unhide any hidden Preparation Properties columns, right-click any column header or row, then on 'Columns', 'Restore Default Column Widths'</p>

Table 5 Run worksheet column properties

Column		Description
Sample Properties	Sample No.	This is a unique number Omnion assigns to each individual sample in the Run. Sample No. is the same as the row number of the spreadsheet. Sample No. cannot be edited.
	Cup No.	This is the number of cups or sample tubes within the sample rack where the sample is or will be placed. Cup numbers from 1..n, where n is an integer, refer to the Sample Racks and cup numbers from S1..Sn refer to the blue Standards Rack. A letter "S" needs to be placed in front of the cup number for the sample to be taken from the calibration standards rack. If a Cup No. is not shown in the Racks tab, the Cup No. will not be changed, but when this sample is run, the autosampler will simply ignore the Cup No. by not moving the sample probe to this Cup No. position. For the ASX-400 autosampler which has a single rack, Sn and n refer to the same Cup and are interchangeable.
	Sample ID	Identifies the sample to be run.
	Sample Type	Select the Sample Type most appropriate to this sample. The default is Unknown, all other types are for quality control purposes. The Sample Types available determine the properties of the sample: Unknown, Calibration Standard, Check Standard, Spike Set, Duplicates Set, Spiked Duplicates Set and Method Detection Limit.
	Reps	This is the number of times the sample is injected and analyzed. Reps=1 is the default, the sample must be run at least once. Enter a number between 1–99.
Sample Prep Properties	ADF	Autodilution factor (ADF) can be used if the system has an Autodilutor. If the box to the left of the ADF column is checked, the dilutor will perform a dilution on that sample. Any sample type can request an autodilution. The ADF column is for entering the autodilution factor or amount of dilution for the autodilutor to perform. The box to the left of this column must be checked to enter a number into this field.
	Trigger Off	Trigger Off is for turning off the autodilution trigger for a specific sample. The autodilution is triggered if the determined concentration of a sample is above a specified level. This level is specified in the analyte portion of the run properties window as a percent of the high standard. To turn the trigger off for a specific sample, the trigger must be on for the analyte in question. The trigger for an analyte is turned on in the analyte portion of the run properties window. Trigger Off will automatically be selected for Calibration Standards. If a sample triggers an autodilution, the software will add a copy of the sample line to the end of the Run Worksheet. The added sample will have the ADF box checked and the ADF column will have the autodilution factor that will be used.
	MDF	Manual Dilution Factors (MDF) can be used if the sample was diluted prior to the Run. The column labeled MDF is for entering the manual dilution factor or amount of dilution that has been performed prior to analysis. This column can only be edited if the column to the left is checked.
	Weight	There are three different columns for Weight. The column labeled Weight is for entering the weight factor or amount of sample that has been used in an extraction performed prior to analysis. This column can only be edited if the box to the left is checked. The column labeled Units is for specifying the units of measurement used in weighing the sample.

Run setup

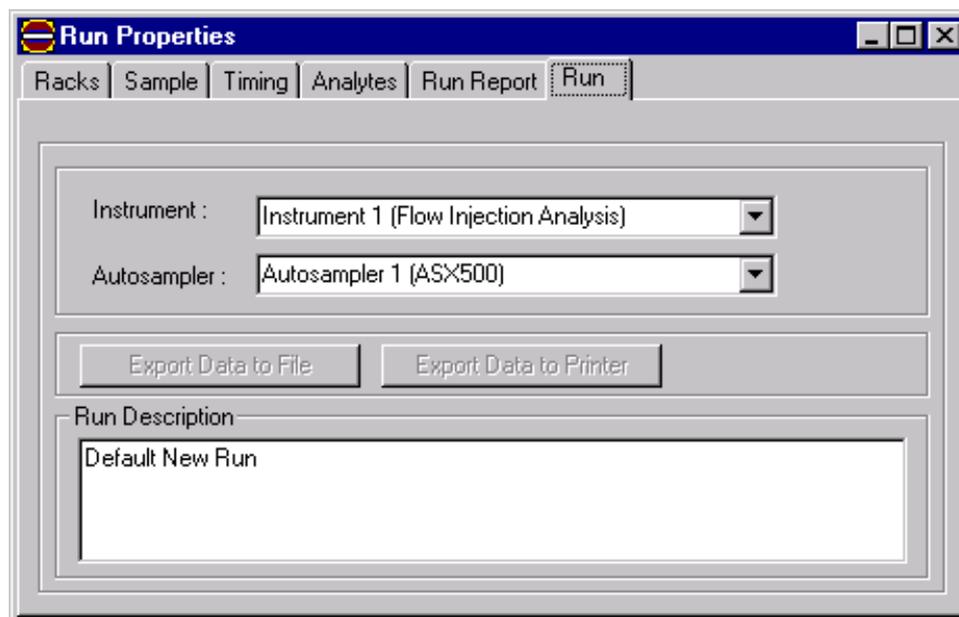
9.1.1 Hiding sample prep properties

If the instrument does not have an autodilutor or does not use one or more of the columns in the Run Worksheet, the columns can be hidden from view.

1. Click the column heading (for example, ADF) to select the entire column.
2. Right-click and select Hide. The columns will be hidden on the Run Worksheet.
3. To view the hidden columns, select any column header and right-click. Select Restore Default Column Widths.

9.2 Editing the run properties window

Before starting a run, first define the run properties. The Run Properties window includes properties of Samples, the Method, the associated Instrument Configuration and any Data acquired. Each row of the Run Worksheet refers to a Sample. The row columns contain some of the sample properties, but the rest of the Sample properties are found in the Run Properties window.



The Run Properties window has six tabs for the various run properties; Racks, Sample, Timing, Analytes, Run Report and Run. Click the tabs to display the various fields for that property.

9.2.1 Setting the run properties

The **Run** tab sets the instrument and autosampler being used. These settings do not have to be changed if one instrument and one autosampler is used. Export options and a Run description are also entered in the **Run** tab.

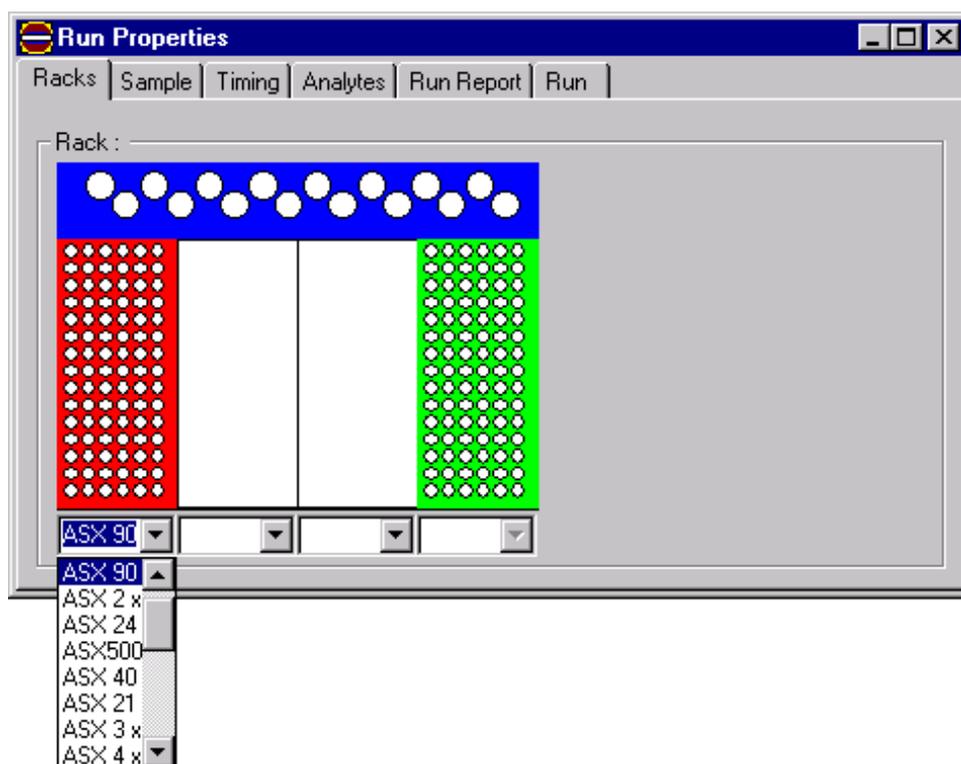
1. From the main menu, select **WINDOW>TILE**. Click the **Run** tab of the Run Properties window,
2. In the Run Description box, remove the existing text and enter a description relevant to the analysis being performed.

9.2.2 Setting the sample rack properties

The **Racks** tab shows the geometric layout of the autosampler tray. This design was selected in the Configuration screen. The standards and dilution rack types are set in the Configuration. To make changes to the rack types, click **CONFIGURATION>AUTOSAMPLERS** from the Main Menu.

The rack display is used for selecting the desired sample rack for the run. Sample racks will be colored red on the tray screen. The standards and dilution racks will be colored blue and green, respectively.

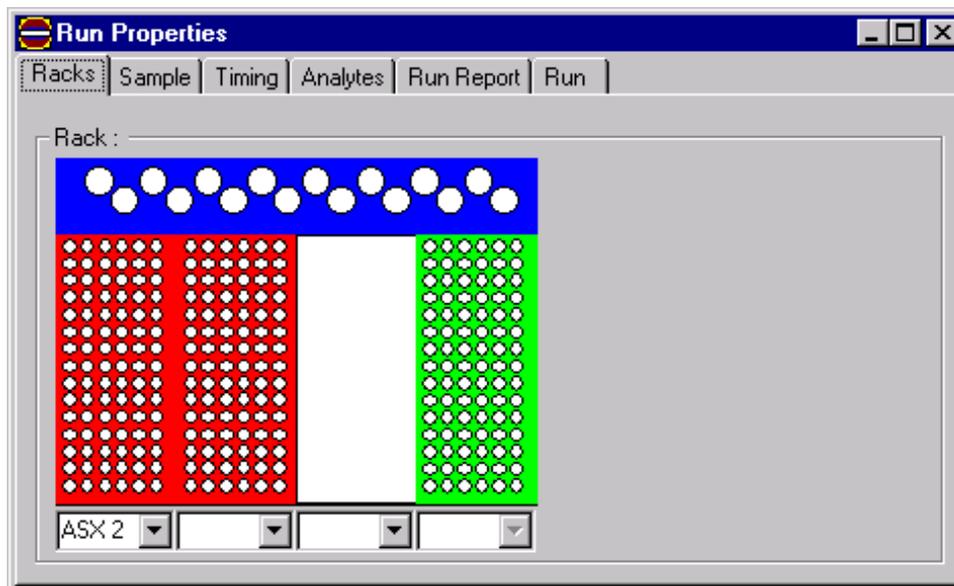
1. Click the drop-down box below the rack to choose the appropriate rack type.



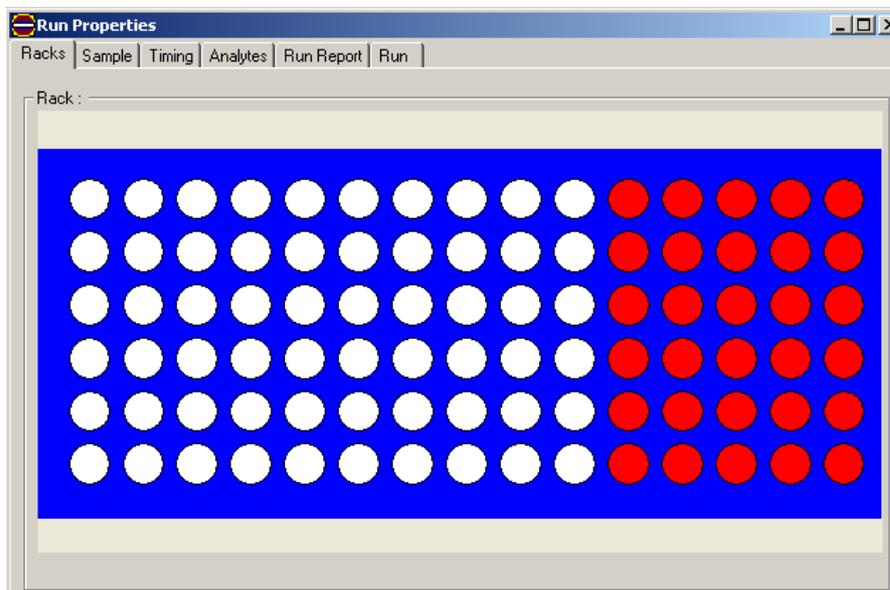
2. After selecting a rack type, the display will automatically change to reflect the new geometric pattern.

Note: A combo rack selection should be made if using more than one slot position. The user will not be able to select individual types to fill each slot position.

3. If more than one sample rack slot is to be used in the tray a combo rack can be selected to cover more than one slot. For example, when using two 90-position sample racks, select the ASX 2 x 90 type under slot 1.



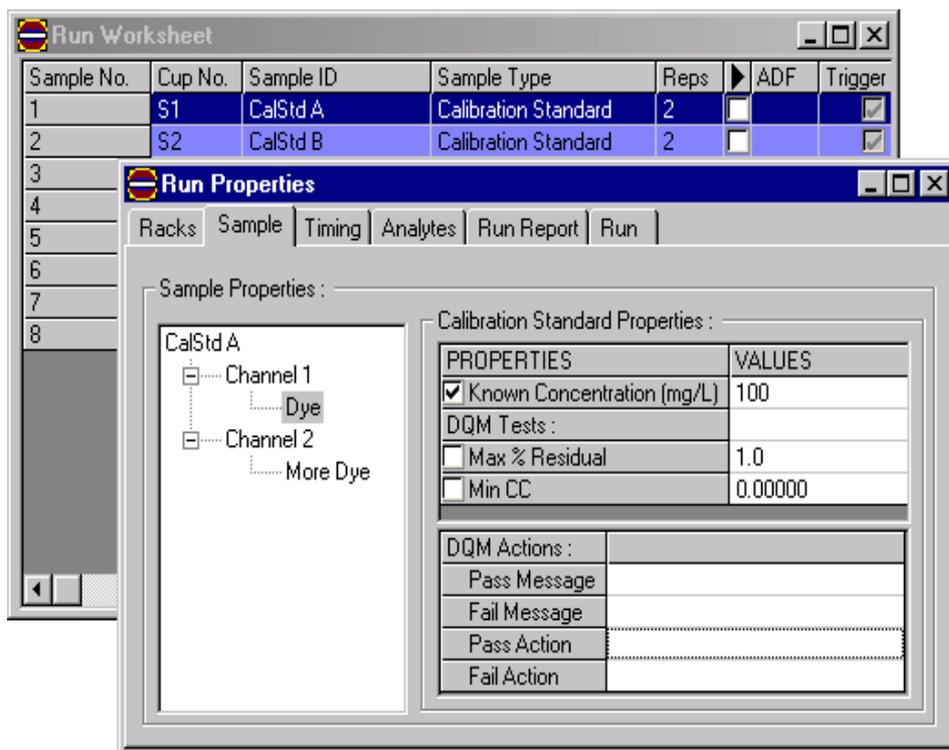
Note: ASX 410 autosamplers have the sample and dilution positions in the same rack.



9.2.3 Setting the sample properties

The **Sample** tab displays the properties for a specific sample selected in the Run Worksheet. In addition, if a specific sample number is selected in the Run Worksheet, the sample properties for that sample will automatically be displayed. The properties visible are dependent on the sample type.

1. Click the Sample Type field in the Run Worksheet. The sample properties for the sample type will be displayed in the **Sample** tab.



2. Define the Known Concentration of the standard selected in the Run Worksheet. All known concentrations need to be defined for calibration and check standards.

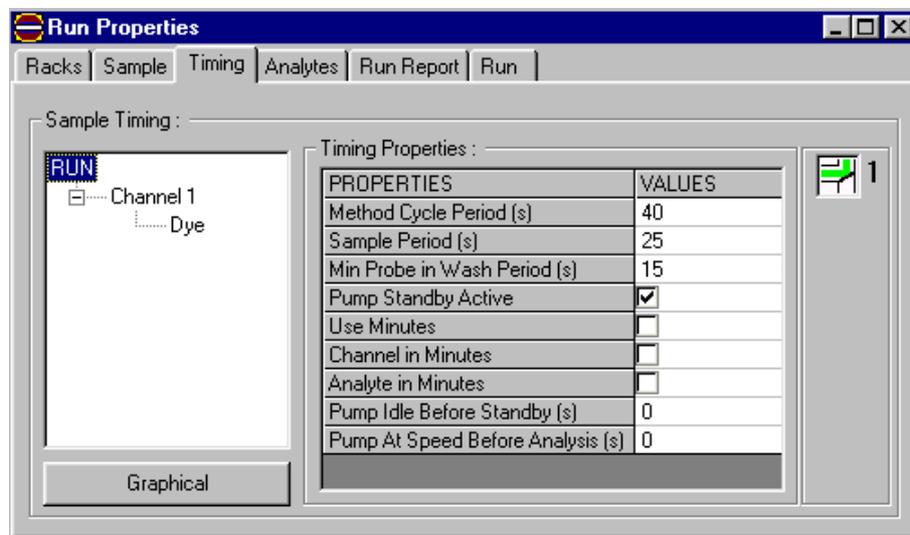
9.2.4 Setting the sample timing properties

The **Timing** tab shows a list of timing and peak detection properties. Some properties apply to all channels, some to specific channels and some only to specific analytes. The parameters to be used are defined in the Lachat QuikChem method. Refer to the Omnion Help File, Run Properties>Timing>Sample Timing for more information on the timing parameters to be used. The Sample timing window is displayed in a tree form, with the root or RUN, branching to each Channel and then each Analyte.

A small box for each channel can be found on the right of the **Timing** tab. The channels are labeled 1, 2, 3, etc. If the valve is in the normal default state (inject) a green path is visible in the box. If the valve is in the load state the path will appear red. Click the box to change the state of each valve. This can only be done with the instrument on.

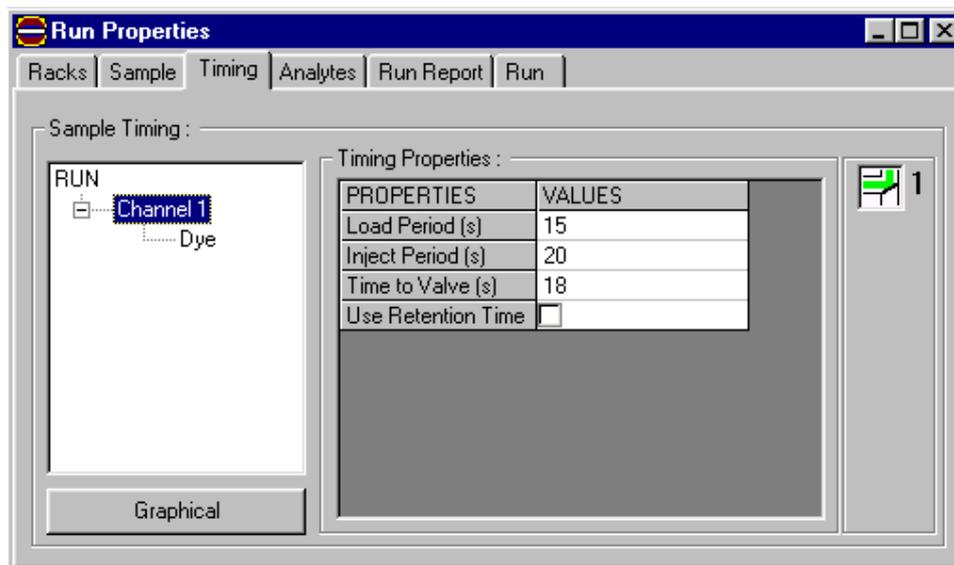
1. Click the **Timing** tab and click **RUN** in the sample timing tree. The timing parameters specific to the sampler will be displayed to the right. See the Omnion Help file, **RUN PROPERTIES>TIMING>SAMPLE TIMING** for more information on these parameters.
1. These parameters are used by the system to control the pump and autosampler. Using appropriate values for the sampler

timing will ensure that the right amount of sample is sent to the instrument at the appropriate times. Other values are used for the pump standby feature. Other options include changing the timing parameter units and channel display units from seconds to minutes. This is commonly done when running ion chromatography.



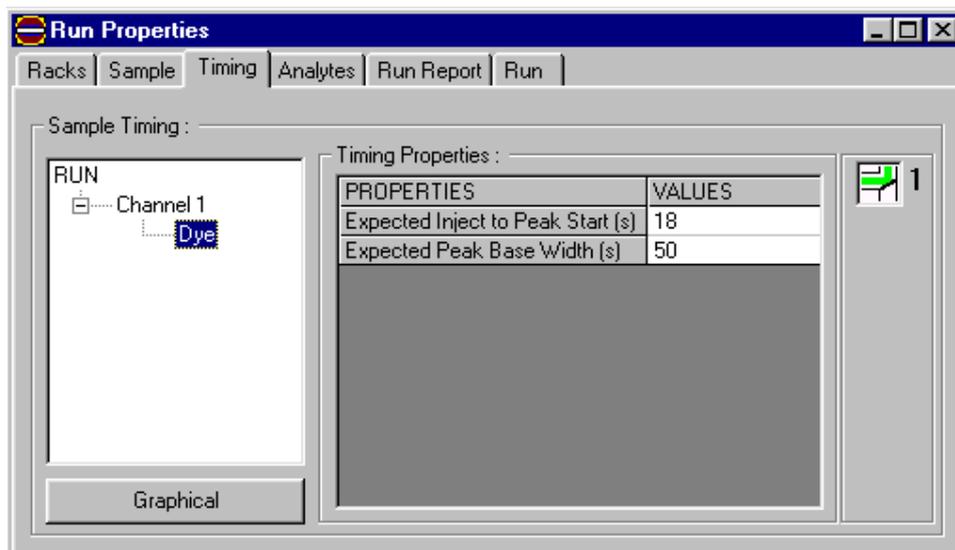
2. Click a channel under Run. The timing parameters specific to the channel will appear. See the Omnion Help file, **RUN PROPERTIES>TIMING>SAMPLE TIMING** for more information on these parameters.

These parameters are used to control the valve for the channel that is selected. Using the appropriate values for Channel timing will ensure that a consistent slug of sample is injected onto the manifold for the channel selected.

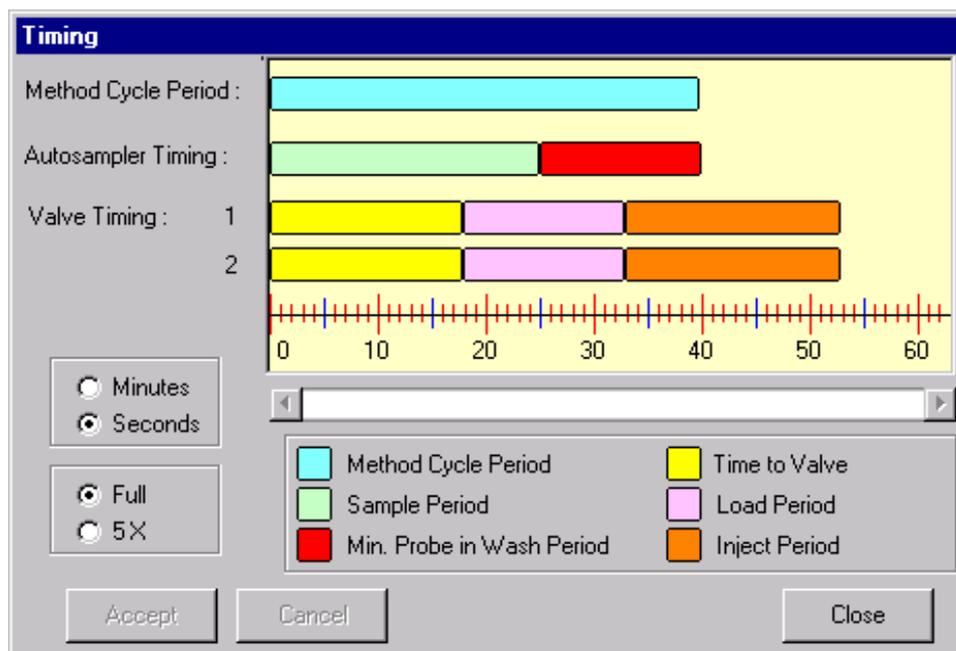


3. Click the appropriate analyte. The timing parameters specific to the analyte will be displayed.

These parameters are used by the system for creation of a peak expectation window needed for peak detection and quantification. Using the appropriate values in analyte timing will ensure that peaks are appropriately detected. Unlike the sampler and channel timing parameters, if the analyte timing parameters are not correct the peak expectation window can be adjusted after the run.



- Click the **GRAPHICAL** button to view a graphical overview of parameters. A window will be displayed, showing how timing parameters work together.

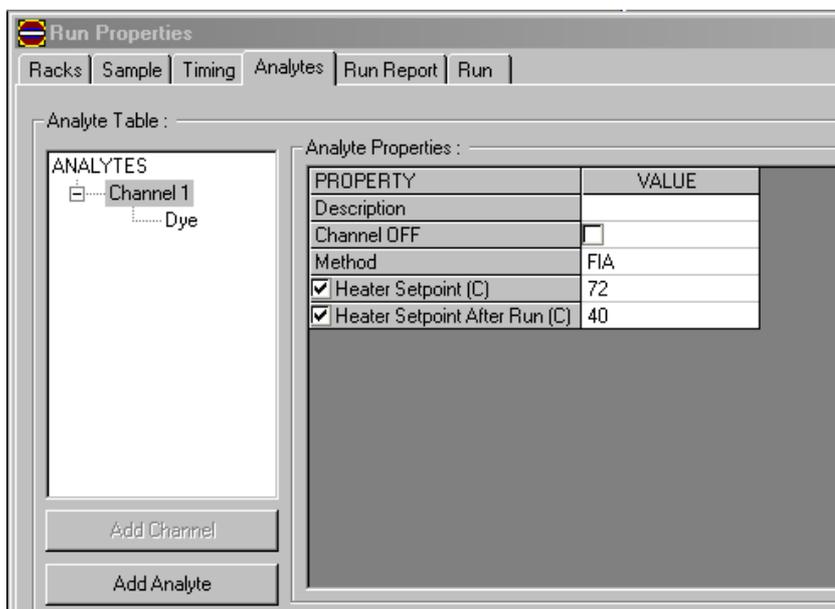


9.2.5 Setting the analyte properties

The **Analyte** tab shows the parameters specific to each analyte. The parameters used are defined in the Lachat QuikChem method.

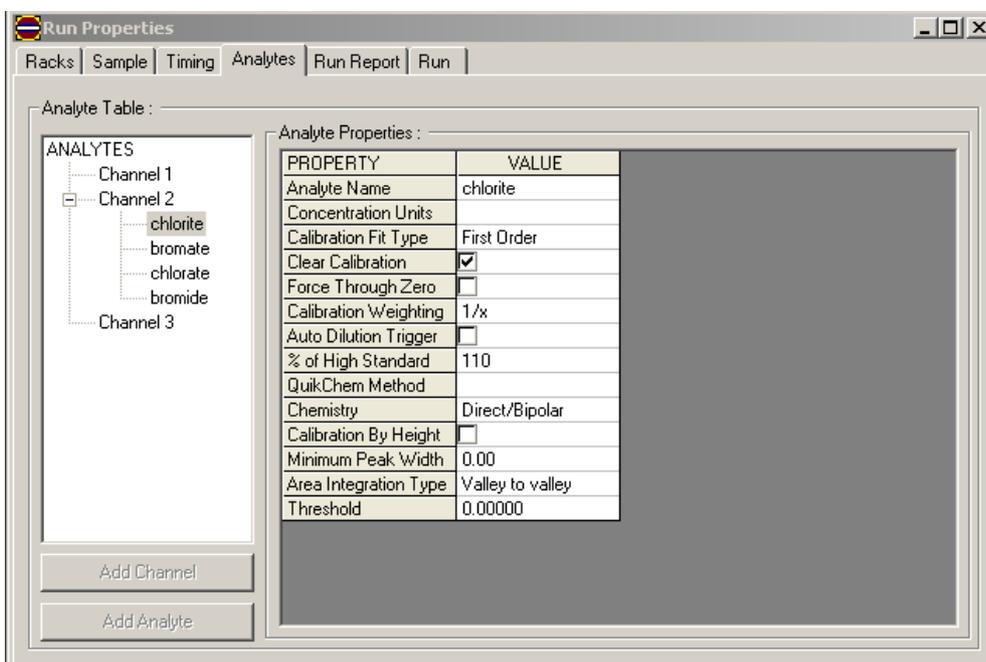
The **Analyte** tab shows how the various analytes are organized under channels, in the form of an analyte tree. Here channels and analytes are added or removed and various channel and analyte properties are defined. Both the **Timing** tab and the **Sample** tab are dependent on this analyte tree.

1. Click the **Analytes** tab. If necessary, enter a description of the channel. The channel can also be turned off for a Multiple Channel Run.



2. Click the appropriate analyte under the channel. The analyte properties specific to that analyte will be displayed. For IC methods, multiple analytes may be shown for a single channel.

Note: Minimum peak width area and area integration type do not apply to FIA methods.

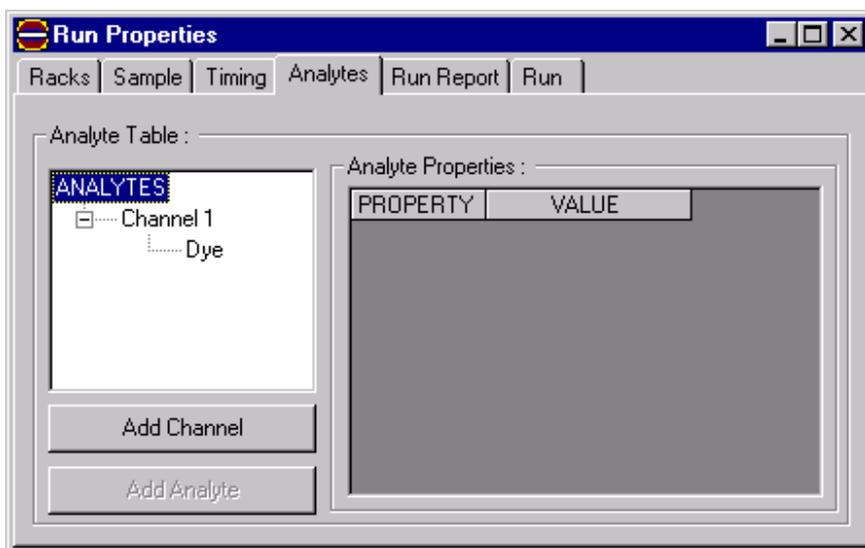


The parameters used are defined in the Lachat QuikChem method. These parameters are used to generate the calibration curve as well as to set the auto dilution trigger when using an automatic dilutor. This trigger applies to samples which exceed the highest calibration standard by the percentage shown in the “% of high standard” field.

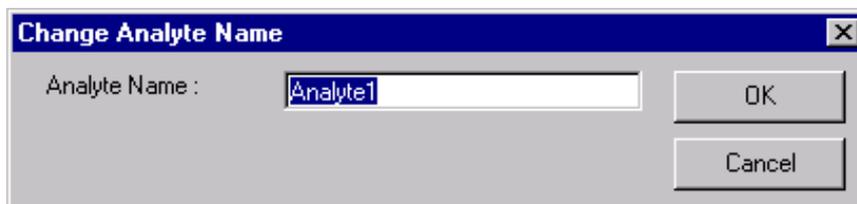
9.2.5.1 Adding channels and analytes

A channel is also referred to as a sample-processing module (SPM). It is a physical component that includes both a valve and detector. The Default New Run begins with one single channel. If multiple channels will be run, additional channels will need to be added. Channels need to be physically attached and configured properly to actually run additional chemistries.

1. Click **ANALYTE** in the Analyte tree. Click **ADD CHANNEL**.

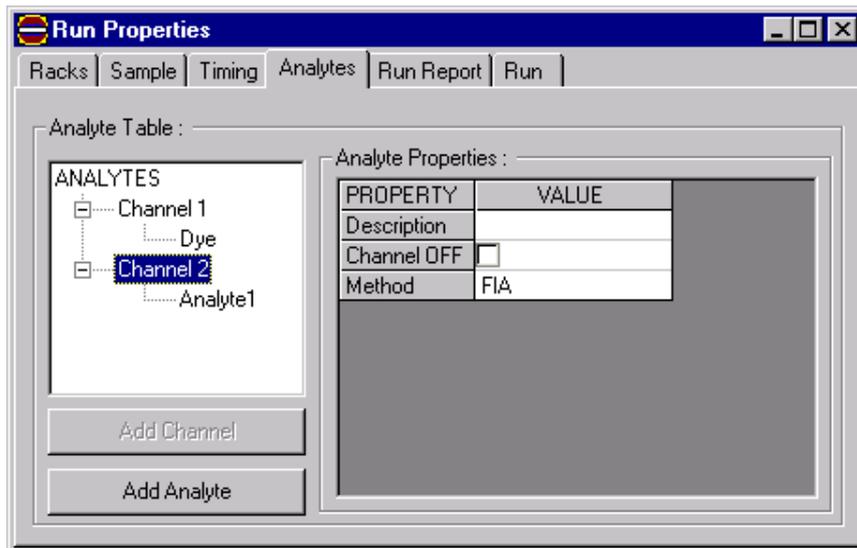


2. A Change Analyte Name window will be displayed. Enter an appropriate name for the analyte.



3. The new channel and analyte will be displayed in the analyte tree.

Note: If the channel has more than one analyte, it is considered an IC channel.

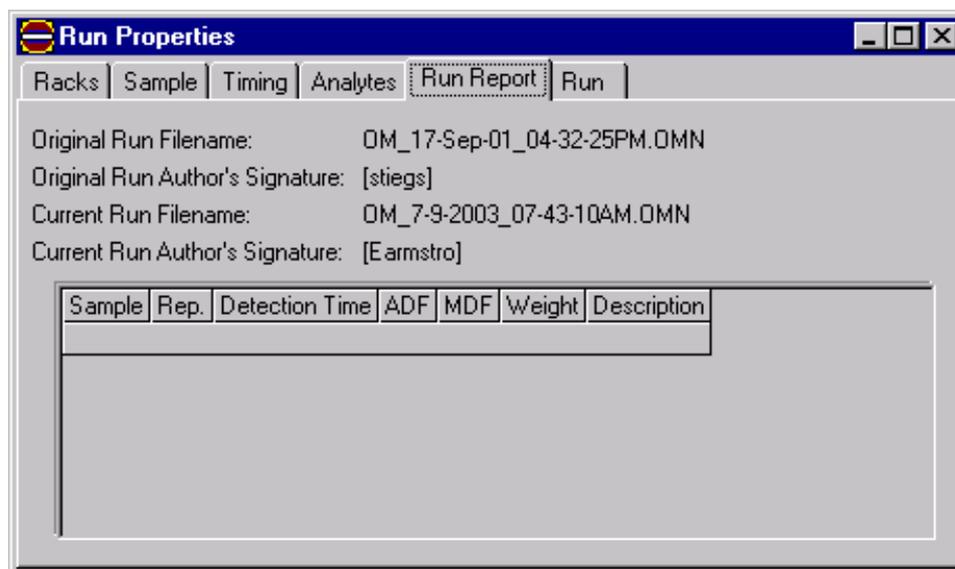


4. Edit the appropriate Run Properties for each channel and analyte.

- To add an analyte to a channel, click the channel and click **ADD ANALYTE**.

9.2.6 Run report

The **Run Report** tab shows the information for the Run currently being viewed. For a run that has not been performed there will not be much information.



9.3 Saving and managing runs

Changes can be permanently saved to the new default run. The saved changes will be part of any New Run created. From the main menu select **RUN>SAVE AS DEFAULT NEW RUN**.

When the file is saved it will use the name at the top of the screen (the date and time at which the Run was started, or the date and time at which a new Run was created). Example: OM_2-19-2003_04-27-21PM.OMN was created at 4:27 on February 19, 2003.

To use this run as a template or to save for another time, select Save or Save As. If Save As is selected, a prompt for a name will be displayed.



To open another Default New Run, click the **NEW** button. The RUN1 and RUN2 buttons will be accessible. Up to four runs can be open at one time. The RUN1, RUN2, RUN3 and RUN4 buttons allows toggling back and forth between the runs that are currently open. Past runs can be reviewed or future runs prepared while a run is in progress. The first run opened will automatically be RUN1, the next will be RUN2 and so on.

9.4 Previewing and starting a run

Start a run after the run worksheet and run properties are set.



To preview the Run before the Run begins, click the **PREVIEW DETECTORS** button. The **PREVIEW** button is a good troubleshooting

tool for reviewing the output from the Detectors and Channels of the Run without running samples or the Run Worksheet.



To submit the Run, click the **START CURRENT RUN** button. The data file does not need to be named, but will be given a name based on the start time and date similar to that described in [Saving and managing runs](#).

9.5 Post-run features

9.5.1 Viewing the channel data display

After a Run is performed, data will be available to view in the Channel Data Display. There will be a Channel Data Display for every channel in the Run.

1. Click the **OPEN** button to open an existing Run.
2. Maximize the Channel Data Display window. There will be one or more peaks for every injection. Each peak has a Peak Integration Window drawn around it (blue box).

9.5.1.1 Click and drag zooming

To enlarge or zoom in to a certain area of the display, click one corner of the area, then drag the zoom box to select the area. Release the mouse button to display only the selected area.

Using this feature during a Run will disable both 'Track Data' and 'Auto Scale'. To restore these, check the box next to each in the Channel Data Display.

9.5.1.2 Zooming buttons



The four buttons at the top left of the display will double (+) or halve (-) the display scaling or sensitivity. There are two buttons for X-Zoom (horizontal) scaling and two buttons for Y-Zoom (vertical) scaling. Click the zoom buttons until the desired view is displayed.

Using the X-Zoom or Y-Zoom controls during a Run will disable Auto Scale but not Track Data. To restore Auto Scale, check the Auto Scale box again.



Click the Restore Full Scale or x1 (multiply by one) button to restore the display to the original autoscaling.

9.5.1.3 Track data and auto scale

The various zoom functions can also be used during a Run. While the samples are being injected and the peaks are being drawn, the scale can be adjusted. The screen is constantly updated and the display will adjust as it continues to acquire further data.

Track data

When the Track Data box is selected, the display will always try to show the active right end of the trace. Track Data is default.

During a Run, using click-and-drag zoom or the scroll bars automatically unchecks Track Data. This will display earlier data without the display automatically returning to the active end of the trace. To restore Track Data, uncheck the box.

The trace will continue to be updated during the Run even if Track Data is not selected; data will not be lost just because it is not visible.

Auto scale

During the Run, when the Auto Scale is checked and the display is refreshed, it will do an automatic x1 (Restore Full Scale). Auto Scale is checked by default. This allows all the data plot to be visible, including the vertical peak annotation.

During a Run, using click-and-drag zoom, the scroll bars or the zoom controls automatically unchecks Auto Scale. This will display earlier data without the display constantly returning to full scale. To restore Auto Scale, uncheck the box.

The trace will continue to be updated during the Run even if Auto Scale is not selected; data will not be lost just because it is not visible.

9.5.2 Viewing calibration results



To view the Calibration Results for each channel analyte(s), click the **CALIBRATION RESULTS** button on the left tool-bar of the Channel Data Display.

There are three sections within the calibration results screen; Calibration Table, Calibration Plot and Calibration Statistics.

9.5.2.1 Calibration table

The Calibration Table provides information for each replicate of each calibration standard run. The numbers in the first column represent each injection. The Known Concentration (mg/L) column, references the concentration from the sample properties for each calibration standard. Other information in the table includes the Rep number, Peak Area (Volts), Peak Height (Volts), % Residual, Date and Time.

The Unused column at the far right side, can be used to remove a Rep from the calibration. If the box in the Unused column is selected, the values in the Calibration Table, Calibration Plot and Calibration Statistics screens are updated to show the effect of removing that replicate from the calibration.

9.5.2.2 Calibration plot

The Calibration Plot shows all of the Reps of the calibration standards plotted on one graph. It plots the analyte peak area or height (y-axis) vs. concentration (x-axis). It also displays a line drawn through those points. This is the calibration curve.

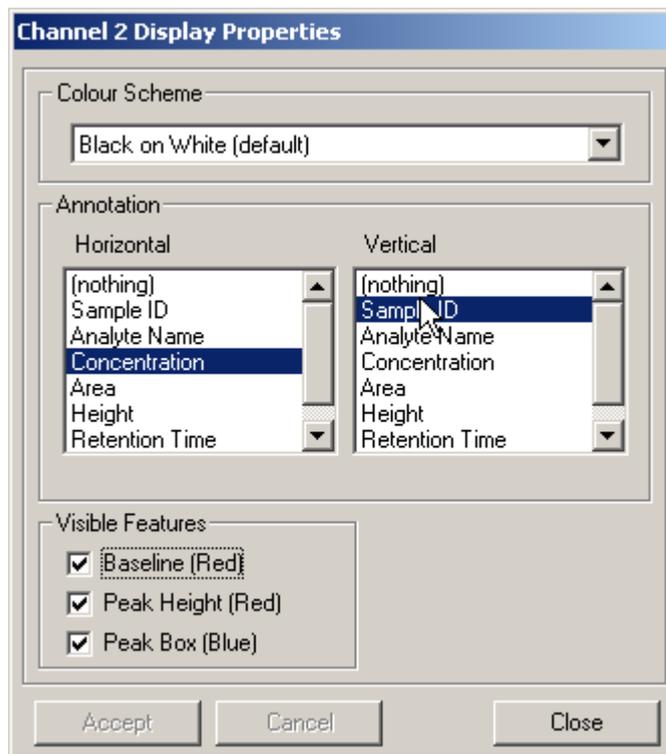
9.5.2.3 Calibration statistics

The Calibration Statistics show the equations and the Correlation Coefficient (r) determined by the calibration curve.

9.5.3 Data editing

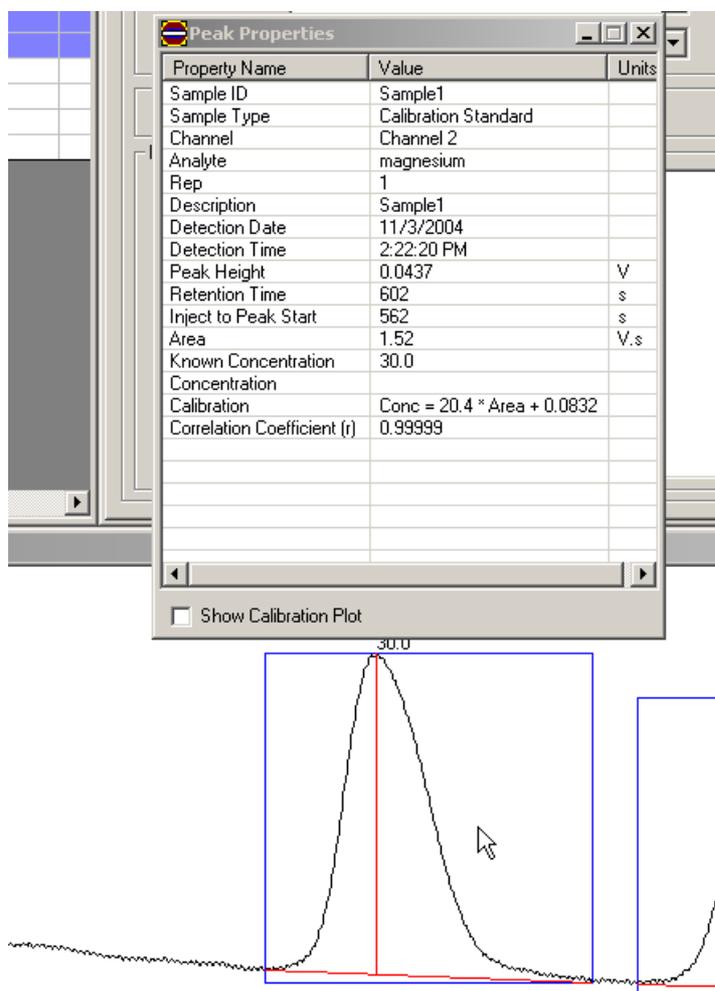
9.5.3.1 Channel display properties

1. Right-click channel data display and select Channel Display Properties.
2. Select Color Schemes. Select one horizontal and one vertical annotation for the sample peak.



9.5.3.2 Peak properties

1. Right-click the channel data display and select Peak Properties.
2. Click inside the integration window to view the properties for the selected peak.

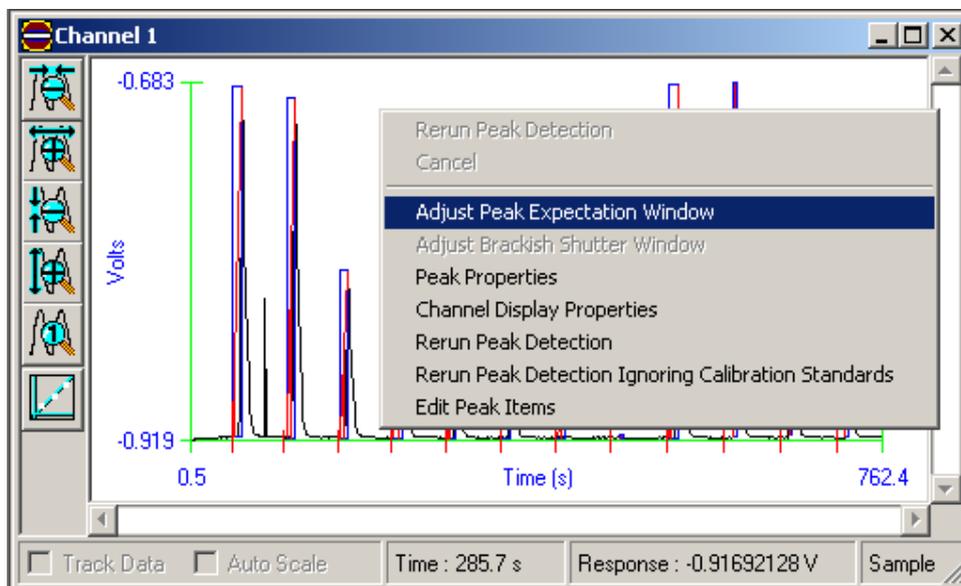


9.5.3.3 Adjusting the peak expectation window and peak detection

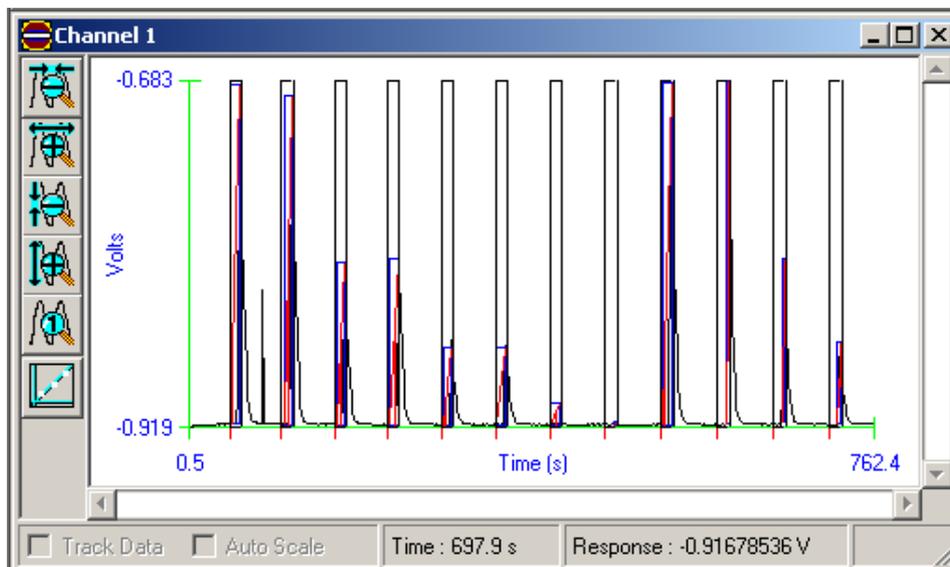
The Peak Expectation Window displays the time boundaries for an expected analyte peak. The Peak Expectation Window is normally invisible. The peak and its baseline (shown in red) cannot begin before the left edge of this box or end past the right edge. The Peak Expectation Window is a property of each individual analyte.

Peak Expectation Windows can and do often overlap each other. However, the peaks themselves never overlap. The peak width or the width of the baseline is detected within the Peak Expectation Windows and is shown inside a blue box.

1. Right-click in the channel data display and select Adjust Peak Expectation Window.



2. The Peak Expectation appears as a blue box, framing the peak.



3. Place the cursor over the Peak Expectation window. Click and drag the Peak Expectation window until it frames the peak to be detected. Adjust the width by clicking and dragging to the right edge.

Clicking and dragging the peak expectation window sets the analyte peak detection parameters for the sample peaks in the Run.

The peak detection must be rerun in order for Peak Expectation window changes to take effect.

4. Right-click the channel data display and select Rerun Peak Detection.

5. Click the **FULL SCALE** button. If the Peak Expectation Window is adjusted correctly, every peak in the run should fall completely within each box.
6. Click **CALIBRATION RESULTS** to view the improved calibration.

9.5.3.4 Edit peak items

1. Right-click the integration window of the peak to be changed.
2. Select Edit Peak Items. From this menu, the sample ID, standard ID or standard concentration can be edited.

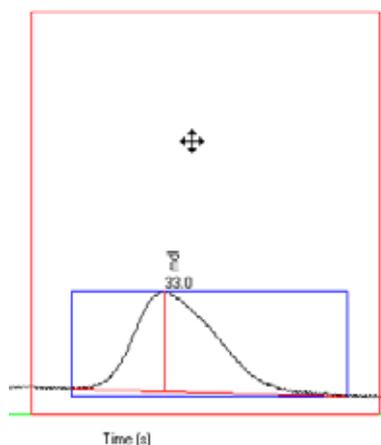
9.5.3.5 Enable threshold mode

1. Right-click the channel data display and select Enable Threshold Mode.
2. Select the IC analyte to be adjusted.
3. Select a section of baseline that is flat and does not have any peaks by holding down the left mouse button and highlighting that section of baseline. The threshold will be entered for that analyte.
4. Right-click again in the channel data display and select Rerun Peak Detection. The software will give peaks less than the threshold setting a “zero” area and use that area in calculating the concentration.
5. Clear the threshold mode by right-clicking on the channel data display and selecting Clear Threshold.

9.5.3.6 Manual integration

1. Right-click the peak of interest in the channel data display and select Adjust Baseline Window for Manual Integration. Click and drag the window to set the baseline for integrating that peak.
2. Right-click and select Run Manual Integration to set the baseline for the peak integration. The window for manual integration will be the same as the baseline window. To reduce the size of the integration window while keeping the same baseline, right-click in the integration box and select Adjust Integration Window for Manual Detection.
3. Click and drag the integration window for the desired integration. The software will integrate the peak between the

beginning and ending points of the integration window and keep the selected baseline for integration.

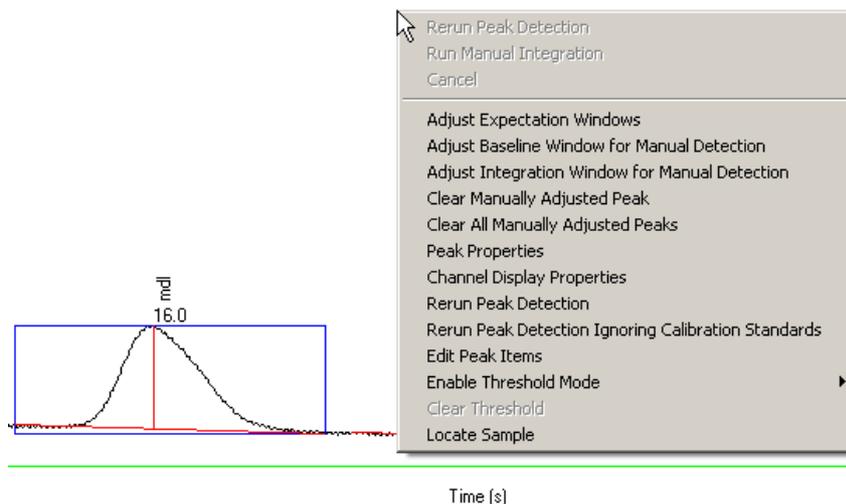


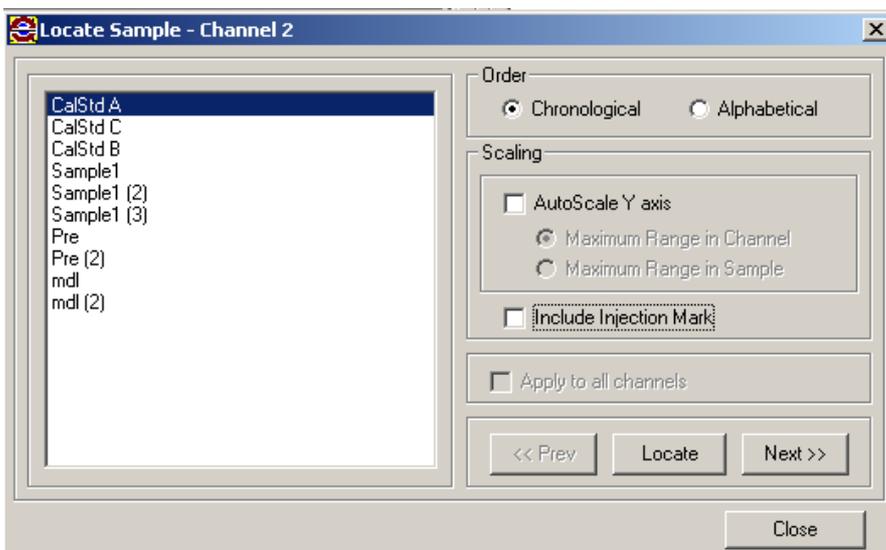
9.5.3.7 Valley to valley and horizontal baseline

Use this feature, located under the **Analytes** tab, when two peaks are located close together with no baseline separation. When Valley to Valley (the default setting) is selected, the integration will occur from the baseline to the valley between the two peaks. If the integration should go to the baseline select Horizontal Baseline.

9.5.4 Sample locator

1. Right-click the channel data display and select Locate Sample. Select a sample to locate.
2. Click **LOCATE** to display the injection data.





9.5.4.1 Injection to injection navigation

Navigation buttons in the lower right hand and left corners on the channel data plot window allow the user to navigate to the next or previous injection and keep the same zoom level.

9.6 Using DQM Check Standard and predefined DQM standards

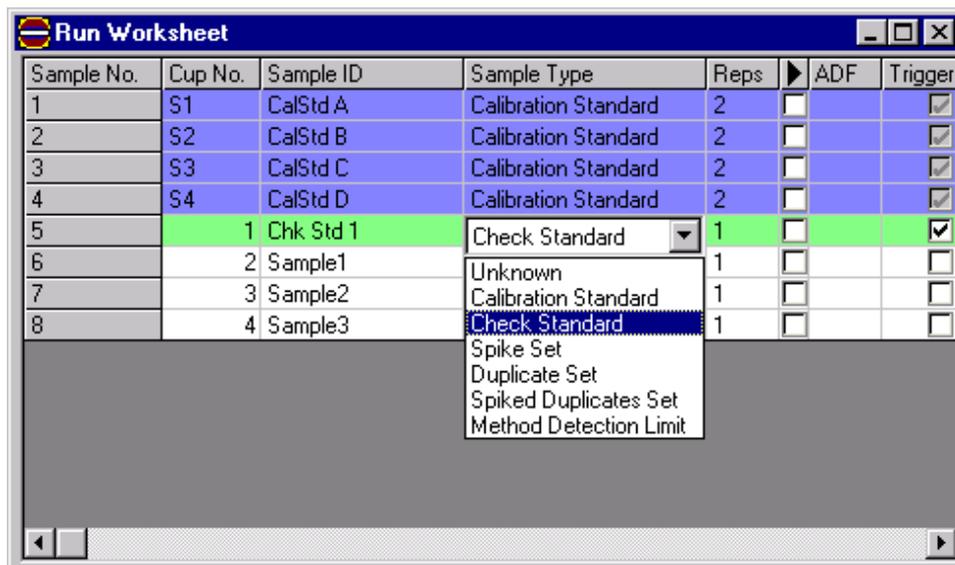
Data Quality Management (DQM) is a powerful tool unique to Omnion. It can implement and document a Quality Control (QC) plan into the Runs. DQM is formed within the Run Worksheet by defining properties of the samples DQM Tests, DQM Pass and Fail Messages and DQM Pass and Fail Actions.

Within the Run Worksheet, collections or sets of DQM samples called DQM sets are defined. This extends the power of individual DQM samples of custom collections of QC samples.

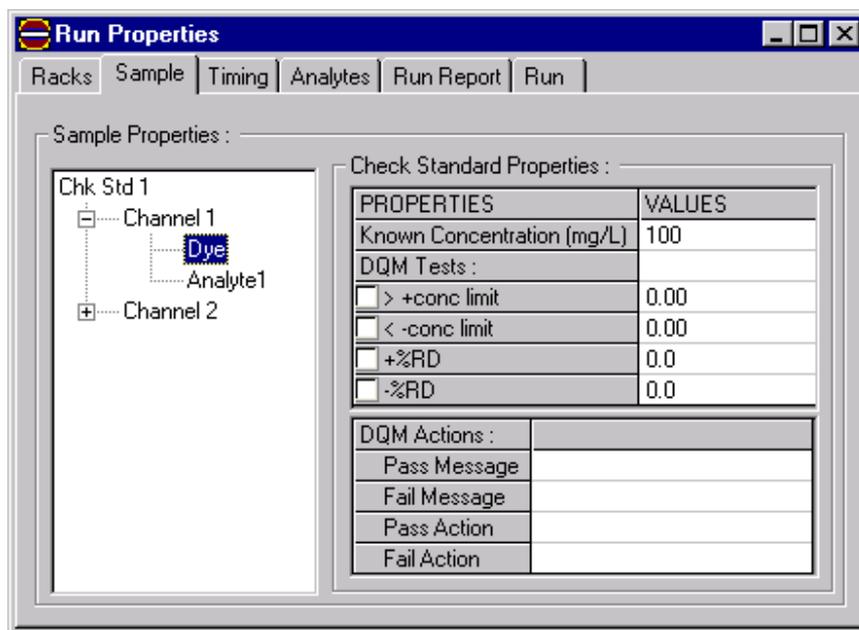
9.6.1 Setting the check standard for sample type

A Check Standard is a common DQM sample type. Check standards are often included at various points in a run to verify that the calibration is accurate. A check standard is simply a standard of a known concentration run to check that a correct value is obtained. The known concentration and one or more DQM tests will define the correct value. The tests can also be relative, meaning the determined concentration must be within a specified percentage (above or below) of the known concentration. The Check Standard Sample Type is also used for blank checks. In the case of checking blanks, the known concentration is zero.

1. Select the appropriate field in the Sample Type column. A drop-down arrow will appear. Click the drop-down arrow and select Check Standard.



2. Click the **Sample** tab in the Run Properties window. Click the analyte directly under the channel. The check standard properties for the analyte will be displayed. The first value is Known Concentration.



3. Select Known Concentration to edit the value.
4. Set the DQM tests to the check standard (see [Table 6](#)). Check the appropriate DQM test and set the values for the limits.

5. Set the DQM actions. See Section 9.8.1 on page 72 for more information on setting DQM actions.

Table 6 DQM tests for sample type check standard

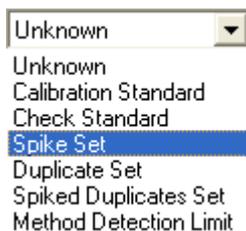
	DQM Test	Definition
Absolute Check Standard	> +concentration limit	If the determined concentration of the Check Standard is greater than the value entered, the Fail Message will be given, and the Fail Action will be taken. If the determined concentration is less than the value entered, the test passes: the Pass Message will be given and the Pass Action is done. Note that the value entered here for the test limit is the actual concentration limit, not the difference from a Known Concentration. For example, if the Known Concentration is 100 mg/L, and the test limit is 10 mg/L greater than this, enter '110 mg/L' as the test limit.
	< -concentration limit	If the determined concentration of the Check Standard is less than the value entered here, the Fail Message will be given, and the Fail Action will be taken. If the determined concentration is greater than the value entered here, the test passes: the Pass Message will be given and the Pass Action is done. Note that the value entered here for the test limit is the actual concentration limit, not the difference from a Known Concentration. Example 1, if the Known Concentration is 100 mg/L, and the test limit is 10 mg/L less than this, enter '90 mg/L' as the test limit. Example 2, if > +conc limit = 100 and < -conc limit = 80, if the Check Standard's determined concentration was 90, both tests would pass because 90 is within the range 80 to 100. If the Check Standard's determined concentration was 110 or 78, one test would fail because both 110 and 78 are outside this range. These two separate DQM Tests and values determine different positive and negative limits.
Relative Check Standard	+%RD (% Relative Difference)	If the determined concentration of the Check Standard is greater than the percent difference value entered here, the Fail Message will be given, and the Fail Action will be taken. If the determined concentration is less than the percent difference value entered here, the test passes: the Pass Message will be given and the Pass Action is done.
	-%RD	If the determined concentration of the Check Standard is less than the percent difference value entered here, the Fail Message will be given, and the Fail Action will be taken. If the determined concentration is greater than the percent difference value entered here, the test passes: The Pass Message will be given and the Pass Action is done. %RD is defined as: $100\% \times (\text{Determined concentration} - \text{Known concentration}) / \text{Known Concentration}$. If the Known Concentration = 0.00, the Check Standard is known as a 'blank', and no %RD can be calculated. These two DQM Tests will always pass for a blank. Notice that %RD has a sign to it. To test a negative -%RD, enter it as a negative number. For example, for a 'pass range' of $\pm 10\%$, set +%RD = 10% and -%RD = -10%. If the Known Concentration is 100, and the Check Standard's determined concentration was 90 or 110, -10% or +10%, respectively, both tests would pass. If it was instead 117 or 78, +17% and -22%, respectively, both tests would fail. The Pass Message for both tests could read "Check Standard within 10% of 100". These two separate DQM Tests and values define different positive and negative limits.

9.7 Setting predefined DQM sets

The Sample Types Spike Set, Duplicate Set, Spiked Duplicated Set and Method Detection Limit are all predefined DQM sets. When these sample types are selected in the Run Worksheet, more than one sample is inserted to form a set of samples that act together to perform a DQM function.

For example, the Sample Type Spike Set creates a DQM set for two samples: Unspiked and Spiked. The Sample Type Method Detection Limit creates, by default, a set of 7 replicates of the same sample.

Predefined DQM Sets can be copied and pasted by selecting all or just the first rows. They can only be copied/pasted as a whole set; they cannot be divided.



1. Click the appropriate field in the Sample Type column. A drop-down arrow will appear in the right side of the field.
2. Select a predefined DQM set from the drop-down menu. The selected DQM set will be highlighted for easy identification from the rest of the samples in the tray. See [Table 7](#) for more information on the predefined DQM sets.
3. If necessary, renumber the cups and enter the appropriate Sample ID.

Table 7 Predefined DQM sets

Predefined DQM	Definition
Spike Sets	<p>Spike Sets can be used to define a set of two samples, “Unspiked” and “Spiked” which, when both run, will give information on spike recovery. This recovery is used to reveal matrix effects on the determination of this analyte from a real sample matrix. The matrix includes everything in the sample except the Analyte, i.e., the solvent (usually water) and everything dissolved or suspended in it.</p> <p>A Spike Set is made by adding an amount of concentrated solution containing the analyte, or the Spiking Solution to one of two sample replicates to form the spiked sample. Generally, the dilution effect of the addition is neglected if the volume of added spiking solution is less than 1% of the total spiked sample volume. The Spike Set then consists of the original Unspiked sample and the Spiked Sample. Both samples must be run as a set to obtain the spike recovery. In a Spike Set, the determined concentration of the added analyte divided by the known concentration of the added analyte, times 100% is the percent recovery.</p>
Duplicate Sets	<p>Duplicate sets are run to check precision. By running the same sample twice, the results obtained can be compared and tested whether or not they fall within an acceptable difference of each other. The set consists of two samples, Duplicate 1 and Duplicate 2. The duplicate set can be evaluated using the Maximum Relative% Difference or the Maximum Conc. Difference.</p>
Spiked Duplicate Sets	<p>A Spiked Duplicates Set is a convenient combination of the Spike Set and the Duplicates Set, but using a total of only three samples. The first sample takes on the role of the 'Unspiked' sample. The second sample, 'Spiked 1', takes on the role of the Duplicate 1 sample. The third sample, 'Spiked 2', takes on the role of both the Spiked and the Duplicate 2 sample. Thus, 'Spiked 1' and 'Spiked 2' are the duplicate samples.</p>
Method Detection	<p>The Method Detection Limit (MDL) sample is a single sample run, by default, seven times. It is usually chosen to be at or near the lowest calibration standard concentration, but must be greater than 0.00.</p> <p>The MDL is in the units of analyte concentration and is an estimate of the minimum, non-zero concentration which can be determined by the method given its precision near (but not at) zero concentration. There are over a hundred definitions of the lower non-zero concentration limit of a method. Here we use the MDL as defined by the U.S. Environmental Protection Agency (1984. “Definition and procedure for the determination of method detection limits.” Appendix B to 40 CFR 136 Rev. 1.11. Amended June 30, 1986. 49 CFR 43430.)</p> <p>The USEPA defines the MDL as follows: MDL = Standard Deviation of 7 Replicates x 3.14 3.14 = the T-value for 7-1 degrees of freedom and a 99% confidence interval. The Replicates field can be changed to be a number other than 7. However, the DQM Test will then not calculate the MDL as defined by the USEPA.</p>

9.8 Setting user-defined DQM sets

Note: When editing the Run Worksheet, if all or part of a DQM Set is included in a selection, some restrictions apply to the Run Worksheet's editing commands. Right-click a selection, and if a command appears inactive, then there is probably part of a user-defined DQM Set in the selection and the command is not allowed. Remember that no sample properties within a DQM Set can be edited. Also, the rows within a set cannot be separated.

Some users may want to create their own DQM sets or may want to run a particular set at a regular interval, (e.g., every 10 samples).

Up to 9 DQM Sets, Q1 to Q9 can be defined.

1. Enter the individual samples, of any Sample Type other than Unknown, into one or more rows in the Run Worksheet.
2. Click and drag to select these rows. Right-click within these sections, select Define DQM Set. Select Once, After every N samples or At end of run and click **OK** (see [Table 8](#)).
3. A DQM Set icon will appear to mark the location of the new DQM Set.

Q1

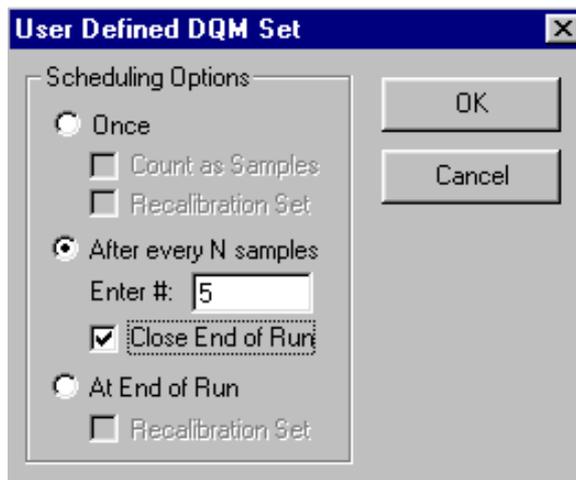


Table 8 User-defined DQM set

Scheduling Options	Description
Once	Runs the DQM Set once, at its current position in the Run Worksheet
	Count as Samples: Samples to be counted by another, repeating DQM set, one with an After Every N Samples schedule.
	Recalibration Set: Defines the DQM Set as the Recalibration Set. This will be the DQM Set referred to in the DQM Actions "Run Recalibration Set", "Repeat and Run Recalibration Set" or "Continue". Note that samples do not have to be limited to the type Calibration Standard within a Recalibration Set.
After Every N Samples	Select this to run the DQM Set after every N samples, where N = 1 (the total number of samples in the Run Worksheet). Enter the value for N in 'Enter Number (#)'. If 'Close End of Run' is selected, the DQM Set will always be run again at the end of the Run, regardless of the value of N. This ensures that all samples are 'bracketed' by this repeating DQM Set. This repeating DQM Set will start at the current row in the Run Worksheet, so make sure this first occurrence of the DQM Set is in the correct row before setting its schedule. Only one repeating DQM Set is allowed in a Run Worksheet.

Table 8 User-defined DQM set (continued)

Scheduling Options	Description
At End of Run	Select this to run the DQM Set once, but always at the end of the Run. The end of the Run may change as reruns or repeated samples are scheduled during the Run. This ensures that this DQM Set will always be the last thing to run.
	Recalibration Set: Defines the DQM Set as the Recalibration Set. The Recalibration Set will then always be at the end of the Run. This may be useful if no calibration will be performed at the start of the Run, but the DQM Actions "Run Recalibration Set" and "Repeat/Continue" will be used.

9.8.1 Setting DQM actions

DQM Actions define the Pass Message and Fail Message for a DQM test. DQM Actions also define the Pass Action and Fail Action. The DQM Actions include Stop Run, Run Recalibration and Repeat, Run Recalibration and Continue and Continue. See [Table 9](#) for more information on DQM Actions. The DQM Actions listed in [Table 9](#) are ordered from least to most severe.

Each DQM Test has its own independent set of Pass/Fail Messages and Actions.

1. Click a DQM Test. To make the display easy to read, a set of only four DQM Messages and Actions are shown, for the selected DQM Test.
2. If the DQM Test is active, the box is checked and the name of the DQM Test will appear above the DQM Messages and Actions. If the DQM Test is inactive, the box is not checked, no name will appear and the Messages and Actions cannot be edited.

PROPERTIES	VALUES
Known Concentration (mg/L)	100
DQM Tests :	
<input checked="" type="checkbox"/> > +conc limit	0.00
<input type="checkbox"/> < -conc limit	0.00
<input type="checkbox"/> +%RD	0.0
<input type="checkbox"/> -%RD	0.0
DQM Actions : > +conc limit	
Pass Message	
Fail Message	
Pass Action	
Fail Action	

3. Enter the Pass Message and Fail Message for the DQM Test.
4. Enter the Pass Action and Fail Action for the DQM Test.

If more than one Action should occur for more than one DQM Test, only the most severe Action occurs. For example, if one DQM Test results in the DQM Action Continue and another results in Stop Now, Stop Now is done.

In many cases, all the tests will not need to give Pass or Fail Messages and DQM Actions. By default, the messages are set to be blank, and the actions are set to the default **Continue**. However, if a DQM Test is active, even if the Pass/Fail Message is blank, the messages Pass and Fail will be displayed, respectively.

Table 9 DQM actions

DQM Action	Description
Continue	Default Action. Least severe and means go to the next sample. This is a useful Action to log a Pass or Fail Message. If the Action is left blank, this Action is called 'None' and has the same effect as 'Continue'.
Run Calibrate Set and Continue	This Action will cause the DQM Recalibration Set to be copied and run just after the sample. After the Recalibration Set is run, the run will continue with the next sample following the Recalibration Set. If there is no Recalibration Set defined, the Action becomes the default 'Continue'. When a sample has this DQM Action, the Run will Pause when the last Replicate of the sample is started so that the sample's peaks can be detected. DQM tests will occur and a DQM Action taken based on the results of the sample, or the average results of all Replicates of the sample.
Run Recalibration Set and Repeat	This DQM Action is intended for use only with samples which are within a repeating DQM Set, one with a DQM Schedule 'After Every N Samples'. This action will cause the DQM Recalibration Set to be copied and run just after the sample. Then, all samples between this occurrence of the sample and the previous occurrence of the sample in the repeating DQM Set will be copied and run just below this Recalibration Set. This will include any DQM Sets, marked as Count as Samples or not. This fulfills a common quality control requirement that all samples must be bracketed by Check Standards that have passed their DQM Test or Tests. If the sample requiring this Action is in the first occurrence of the DQM Set, or if the sample is not within a repeating DQM Set, the Action becomes instead 'Run Recalibration Set and Continue'. If there is no Recalibration Set defined, the Action becomes instead 'Continue'. When a sample has this DQM Action, the Run will Pause when the last Replicate of the sample is started so that the sample peaks can be detected. DQM Tests will occur, and a DQM Action taken based on the results of the sample, or the average results of all Replicates of the sample. Since this Action implies that there was something wrong which called for a recalibration, there is a limit on the number of times this action is allowed to occur. Otherwise, if the Action occurs because of repeated DQM Test failures, the Run could continue indefinitely, running the same samples over and over. This limit is defined in CONFIGURATION>OPTIONS> RUN TIME TAB in Maximum Recalibrate / Fail Actions. The default is two recalibrations. When the limit is exceeded, this Action becomes Stop Now.
User Decides	This DQM Action pauses the Run and offers the choices 'Resume' (Continue) or 'Stop Now'. Select this DQM Action only if the instrument will be attended during the Run. Once this menu appears, the Maximum Idle Time begins to elapse. This limit is defined in CONFIGURATION>OPTIONS> RUN TIME TAB in Maximum Recalibrate / Fail Actions. When this period is over, the 'User Decides' Action becomes a 'Stop Now'. This allows time to choose between these two actions. When a sample has this DQM Action, the Run will Pause when the last Replicate of the sample is started so that the sample peaks can be detected. DQM Tests will occur, and a DQM Action taken based on the results of the sample, or the average results of all Replicates of the sample. If more than one Run is active, this User Decides dialog only appears when the Run is selected.
Stop Now	This DQM Action stops a Run immediately. This is the most severe DQM Action. When a sample has this DQM Action, the Run will Pause when the last Replicate of the sample is started so that the sample peaks can be detected. DQM Tests will occur, and a DQM Action taken based on the results of the sample, or the average results of all Replicates of the sample. So, since the Run will already have been paused, 'Stop Now' has the same effect as Stop After Current Sample.

Section 10 Custom reports

10.1 Creating custom reports

Any reports generated can be printed or exported. Reports can be exported to an RTF file or HTML file. The RTF files can be opened in MS Word or other software. The HTML file can be opened in an Internet browser such as MS Internet Explorer. [Table 10](#) explains the Custom Report button toolbar functions.

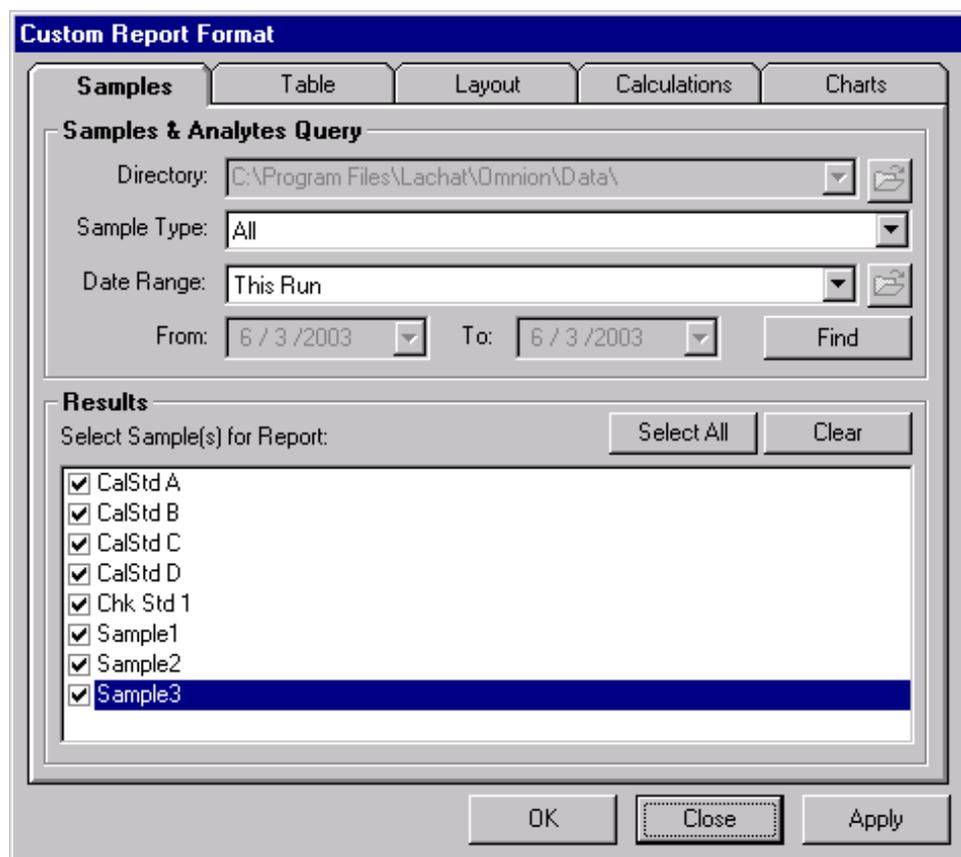
Table 10 Custom report toolbar

Button		Description	Button		Description
	Open Previously Saved Run	Opens a custom report that has been previously saved. If nothing has been created, default is the only selection.		Refresh	Updates the report. Refreshes information in the report if any changes have been to the Run after the report was created.
	Save Format	Saves Custom Report formats. This is very helpful if more that one report format will be used.		Whole Page	Displays the entire page.
	Save as RTF	Exports reports to RTF files.		Multiple Pages	Displays multiple pages on screen.
	Save as HTML	Exports reports to HTML files.		Page Width	Adjusts the size of the page so it takes up the entire width of the display.
	Print Setup	Sets or selects the printer to use. If a printer is not selected, the default printer will be used.		Move to First Page	Moves to the First Page of the report.
	Page Setup	Used to set properties of the page. Adjusts page margins and page orientation.		Move to Previous Page	Moves to the Previous page of the report.
	Print	Sends report to printer.		Move to Next Page	Moves to the Next page of the report.
	Custom report Format	Formats custom reports. Allows changes to the report.		Move to Last Page	Moves to the Last Page of the Report.

10.1.2 Formatting the custom report

The report is formatted using **CUSTOM REPORT FORMAT**.

1. Click the **CUSTOM REPORT FORMAT** button to display the Custom Report Format window.

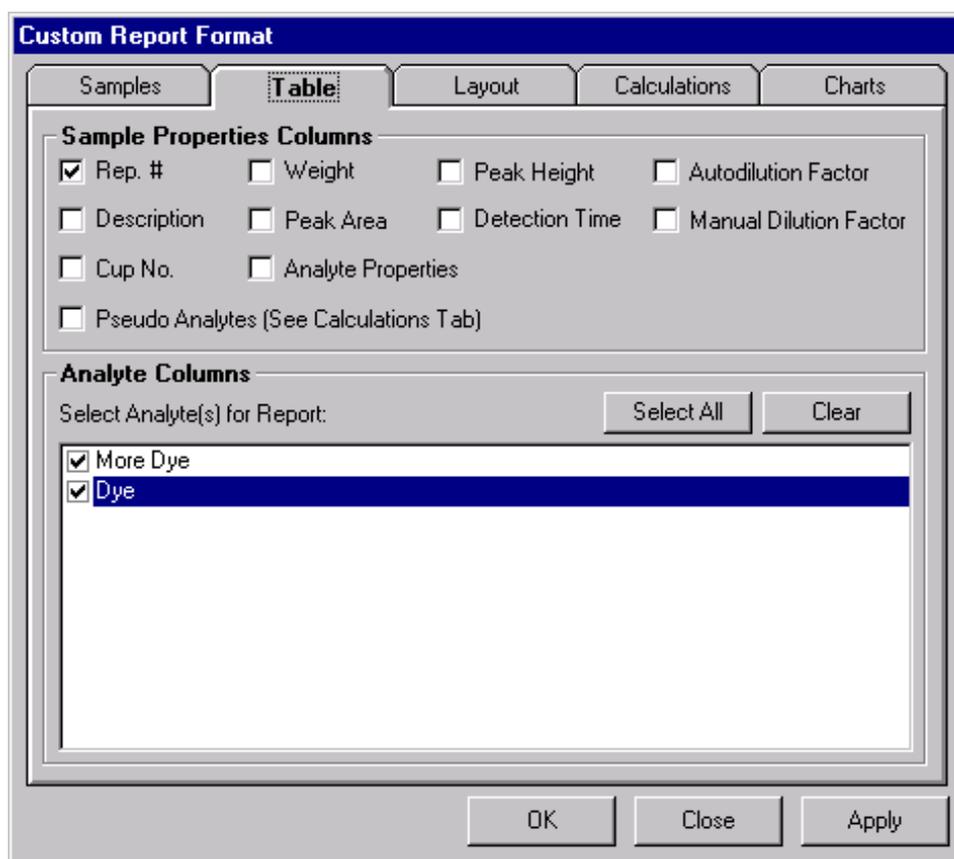


2. Click the **Samples** tab. If necessary, perform a Sample & Analyte Query to determine which samples to display in the report. By default, the report will show samples from the Run that was open when Custom Report was selected.

By performing a query, a report can be generated on samples of a specific type; unknowns, calibration standards or any of the DQM sample types. A query can report samples for a date range; today, past week, month, quarter or year. In addition, custom dates can be selected.

3. Select the Sample Type and Date Range to query from the drop-down menus. Click the **FIND** button to perform the query. The Results will be provided in the Results field.
4. Select or deselect the samples for the report. Click the **SELECT ALL** button to choose all the samples. Click **CLEAR** to delete the selected samples.
5. Click **APPLY** once all the sample selections have been made.

- Click the **Table** tab to set the column properties for the analytes.



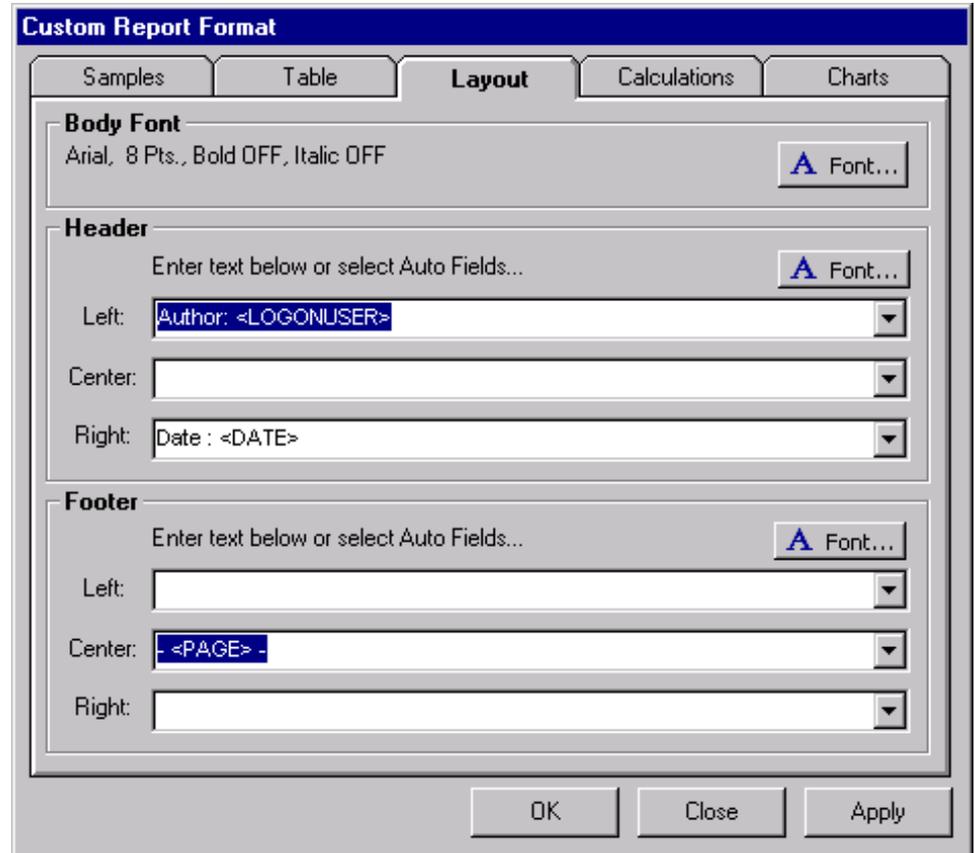
- Select the Sample Properties to add to the report (Table 11). Each new property will create an additional column to the data table of the report for each sample.

Table 11 Sample properties columns

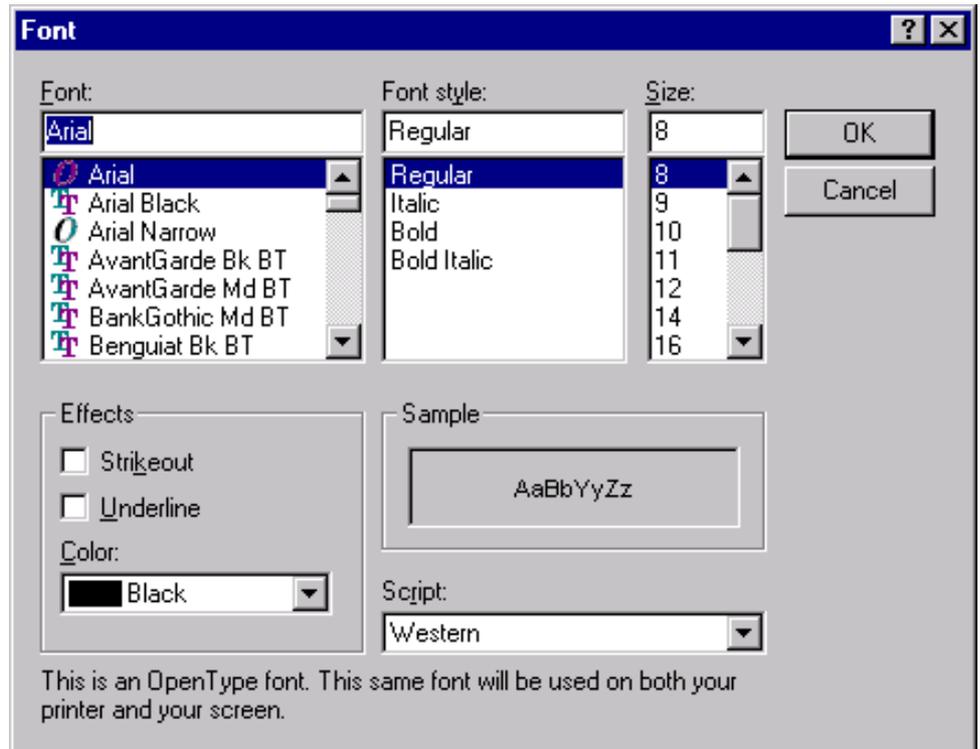
Sample Property	Description
Rep#	Displays the replicate number for that particular sample.
Weight	Displays the weight factors entered in the Run Worksheet.
Peak Height	Displays the peak height for each sample.
Autodilution Factor	Displays any autodilution factors used.
Description	Displays the description entered in the Sample tab in the Run Properties window.
Peak Area	Displays the peak area for each sample.
Detection Time	Displays the time at which the peak was detected.
Manual Dilution Factor	Displays the Manual Dilution factors entered in the Run Worksheet.
Cup No.	Displays the cup number for each sample.
Analyte Properties	Adds a table to the report that gives the properties for each analyte. These are taken from the Analyte tab in the Run Properties window,
Pseudo Channel	Enables the Pseudo-analyte feature in the Calculations tab. Takes the results of two channels and adds, subtracts, multiplies or divides them from each other. For example, this can be used to determine nitrate by subtracting a nitrite channel from a nitrate + nitrite channel or by allowing the subtraction of color or turbidity blanks.

- Select the analytes to be reported.
- Click **APPLY** once all Table changes have been made.

10. Click the **Layout** tab to adjust the look of the report.



11. Click the **FONT** button to change the font properties for body text, header text and footer text.



12. Enter the header and footer information. The header and footer information will be included on every page of the report. Choose to place the information on the left, center or right portion of the page. The information to include is either text or one of the Auto Fields in the drop-down menu. The Auto Fields are Author, Date and Page. Author will give the name of the person who is logged on when the report is created. Date will use the current days date. Page will number each page.
13. Click **APPLY** once all layout changes have been made.
14. Click the **Calculations** tab to set the Sample Preparation, Averages and Pseudo-analytes. Check the appropriate boxes for each field.

The screenshot shows the 'Custom Report Format' dialog box with the 'Calculations' tab selected. The dialog is divided into three main sections: 'Sample Preparation', 'Averages', and 'Pseudo-Analytes'. The 'Sample Preparation' section has three unchecked checkboxes: 'Multiply Concentration by Autodilution Factor', 'Multiply Concentration by Manual Dilution Factor', and 'Divide Concentration by Weight'. The 'Averages' section has two radio buttons: 'Show both Average and Replicates' (selected) and 'Show only Average'. The 'Pseudo-Analytes' section has four radio buttons for 'Analyte #1' through '#4', with 'Analyte #1' selected. Below this, there is an 'Enabled' checkbox (unchecked), a 'Name' field containing 'Analyte 1', and a 'Calculation' dropdown menu. A formula is displayed: 'Formula: Concentration = C1 x X1 (+, -, x, /) C2 x X2 (+, -, x, /) C3 x X3 (+, -, x, /) ... C8 x X8'. At the bottom, there are three buttons: 'OK', 'Close', and 'Apply'.

Sample Preparation							
<input type="checkbox"/>	Multiply Concentration by Autodilution Factor						
<input type="checkbox"/>	Multiply Concentration by Manual Dilution Factor						
<input type="checkbox"/>	Divide Concentration by Weight						
Averages							
<input checked="" type="radio"/>	Show both Average and Replicates		<input type="radio"/>	Show only Average			
Pseudo-Analytes							
<input checked="" type="radio"/>	Analyte #1	<input type="radio"/>	Analyte #2	<input type="radio"/>	Analyte #3	<input type="radio"/>	Analyte #4
<input type="checkbox"/>	Enabled	Name:	Analyte 1	Calculation:	[Dropdown]		
Formula: Concentration = C1 x X1 (+, -, x, /) C2 x X2 (+, -, x, /) C3 x X3 (+, -, x, /) ... C8 x X8							
C1:	[1]	X1:	[None]	C2:	[1]	X2:	[None]
C3:	[1]	X3:	[None]	C4:	[1]	X4:	[None]
C5:	[1]	X5:	[None]	C6:	[1]	X6:	[None]
C7:	[1]	X7:	[None]	C8:	[1]	X8:	[None]
				OK	Close	Apply	

Table 12 Calculations properties

Calculation Property	Description
Sample Preparation	<p>Specify whether the results are to be adjusted by sample prep factors. These include multiplying the determined concentration by the Autodilution or Manual Dilution Factors as well as dividing the concentration by Weight. If any of these are selected, the result in the report will be calculated with these factors figured in. If they are not selected, the report will show the determined concentration of the sample actually injected without calculating in the factors for dilution or weight.</p> <p>It is important to realize that these boxes must be checked so that calculations are done for the results in the report. If the boxes for dilution and/or weight factors in the Table tab of the Custom Report Format window are selected, it will display the factors in the report but will not use them to calculate the results unless they are selected in the Calculations tab of the Custom Report Format window.</p>
Average	<p>Specify whether or not to display the value for each replicate when running samples with multiple reps. The choices are: Show both Average and Replicates or Show only Average. Only one choice can be selected. To display the value for each rep, select the option Show both Average and Replicates. If unconcerned with the value of each rep and are only interested in the average of the reps, select the option Show only Average.</p>
Pseudo-analytes	<p>Takes the results of two channels and adds, subtracts, multiplies or divides them from each other. A common use for this would be in determining nitrate by subtraction. In order to do this we would inject samples on two manifolds at the same time. If a run is made with a nitrate + nitrite manifold on channel 1 and a nitrite only manifold on channel 2, nitrate result can be obtained by subtracting the value for channel 2 from the value for channel 1. In order to use this feature the Pseudo-analytes box must be selected in the Table tab.</p>

15. Click **APPLY** once all Calculations options have been selected.
16. Click the **Charts** tab to configure the Options and Channel Data Displays. Select the appropriate options; Calibration, DQM Tests, Control Chart and/or Channel Data Display. See [Table 13](#) for more information on options.
17. Click **APPLY** once all Chart options have been selected.

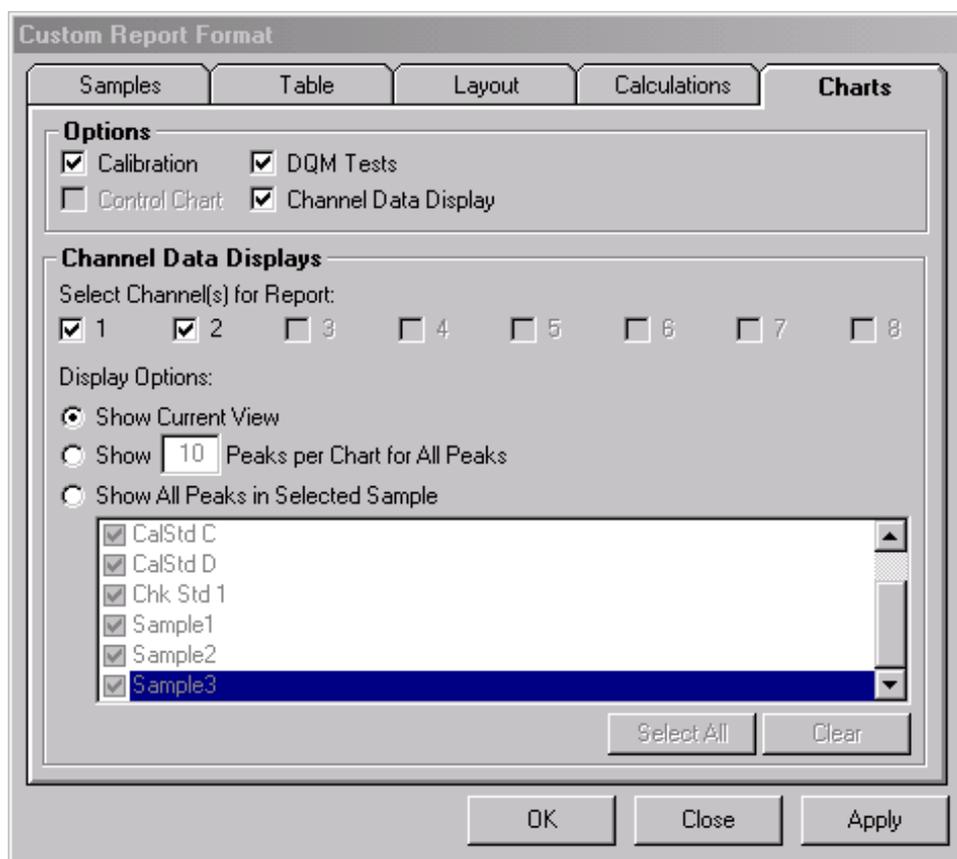


Table 13 Chart properties

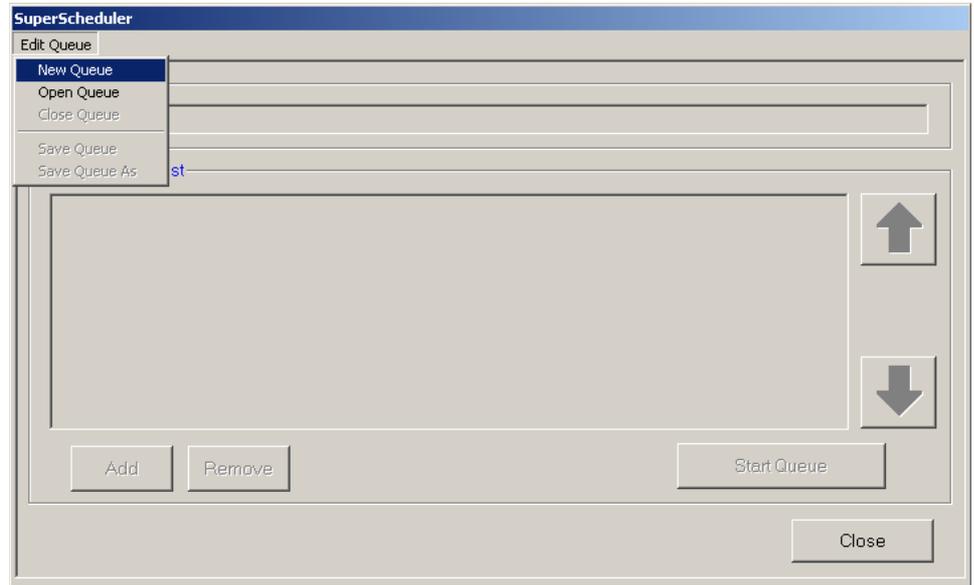
Chart Property	Description
Calibration	Calibration curves will be included in the report.
DQM Tests	Each DQM sample will have an additional row that shows the results of the DQM tests and actions in the report.
Control Chart	This is only available when there is a single sample selected for the report. It is used for plotting the concentration of replicates for a control sample over time. This is likely used after performing a query over some period of time.
Channel Data Displays	Includes the channel data displays in the report. If the Channel Data Displays box is checked, then the options in the Channel Data Displays section becomes active. If the box next to the channel number is checked then the graph for that channel will be included in the report. Click each box to include or exclude any channel's graph.
	Show Current View displays the same graph which is displayed on the screen in the report.
	Show X Peaks per Chart for All Peaks will create as many windows as necessary to display all the peaks in a Run.
	Show All Peaks in Selected Sample displays each sample injected in its own window for each peak. This is useful for Ion chromatology runs where there are multiple peaks for each injection.

Section 11 SuperScheduler

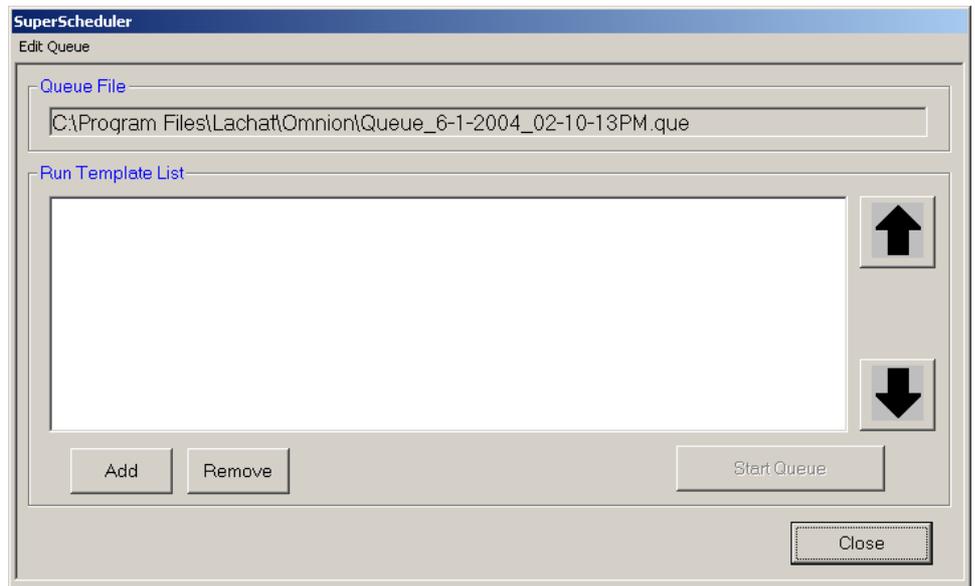
11.1 Using SuperScheduler

SuperScheduler is a tool that allows more than one run to be submitted. When using SuperScheduler, once the first run in the “Queue” is completed, a second run will be started.

1. From the main menu, select **TOOLS>SUPERSCHEDULER**.

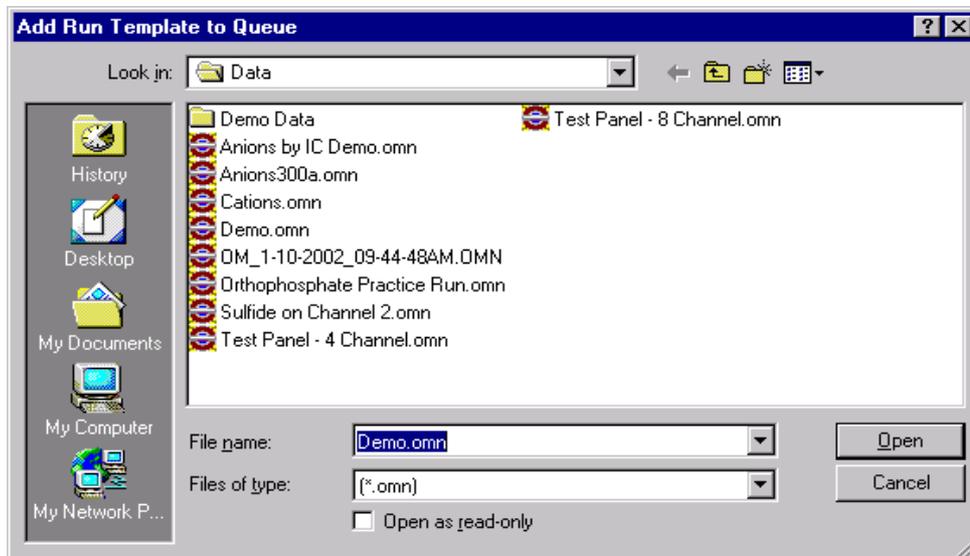


2. Click **EDIT QUEUE** and select New Queue.



3. Click the **ADD** button to enter Runs. The order in which the Runs are added is the order they will run. Use the **REMOVE** button to delete a Run.

***Note:** If run templates are saved in different folders, navigate to find the appropriate folder where the run templates are stored.*



4. Change the order of the Runs using the **UP** and **DOWN** buttons.
5. Click **START QUEUE** to start with the first run template in the list. When the first run is complete, the next run will begin.