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Agilent Technologies

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300/310/320-MS LC/MS and GC/MS Quadrupole Mass Spectrometer MS Workstation Version 6

Software Operation Manual



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Introduction

Overview

MS Workstation Version 6 software controls the 300/310/320-MS Quadrupole instruments, associated Varian chromatography modules and several modules from other vendors. Information in this manual is also on the Help menu.

Additional Manuals

300/310/320-MS LC/MS and GC/MS Hardware Manual

This manual, part number 3954917900, provides information for using, maintaining, and repairing your 300 Series System. This information is also available in Help.

MS Workstation Software Reference Manual

This Manual, part number 391496300, explains the operation of the MS Workstation Software. These operations include displaying and reviewing chromatographic and mass spectral data, library searching, and quantitative analysis. Although these tutorials use Saturn 2000 ion trap files, they illustrate the principles of MS Workstation software.

MS Data Handling Users Guide

This Manual, part number 395403800, provides post acquisition data handling procedures and tasks. These procedures include identifying internal standards, adjusting integration parameters, identifying target peaks, and generating calibration curves.

450-GC User Manual

This manual, part number CP501411, is included on the MS Workstation CD and describes in detail the operation of the 450-GC.

430-GC and 431-GC User Manual

This manual, part number CP501406, is included on the Varian MS Workstation CD and describes in detail the operation of the 431-GC.

DIP/DEP Solids Probe Manual

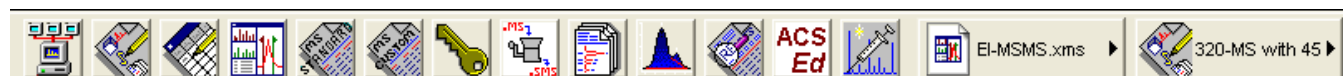
This manual, part number 395414900, which comes with the optional DIP/DEP probe for the 300-MS or the 320-MS GC/MS, describes the operation of the DIP/DEP solids probe.

Workstation Toolbar

Overview

The MS Workstation Toolbar has the following applications: Methods, Data Files, SampleLists, RecalcLists, SequenceLists, and Reports. Installing additional MS Workstation options, such as Star Finder and Star Custom Report Writer, may add other application buttons to the Workstation Toolbar. The following is a brief introduction to the applications. Later sections explain each in detail.

As the cursor moves over a button, the name of the application appears below the cursor. Click an icon to launch the application.



Name of Application	Large Icons	Description
System Control/Automation		Monitor instrument status, and perform automated injections and batch recalculations.
View/Edit Methods		View and edit instrument operation, data acquisition, and data handling methods.
Edit Automation Files		Do off-line editing of SampleLists, RecalcLists, and SequenceLists.
Review/Process MS Data		Review chromatograms and spectra; perform library searches, and review and process quantitation results.
Standard MS Reports		Create, edit, and view standard MS reports.
Custom MS Reports		Create, edit, and view customized MS reports.
Security Administration		Set MS Workstation security options and passwords.
SMS/MS File Conversion		Convert data files between DOS and Windows formats.
Batch Reporting		Generate standard reports for a group of Data Files by dragging and dropping them on the Batch Report Window.
View/Edit Chromatograms		Review GC chromatograms, edit data handling parameters, and recalculate results.
Standard Chrom Reports		Preview standard chromatogram and results reports.
Compound Set Editor		Create and edit sets of compounds in the MS Data Handling Method allowing activation or deactivation under automation.

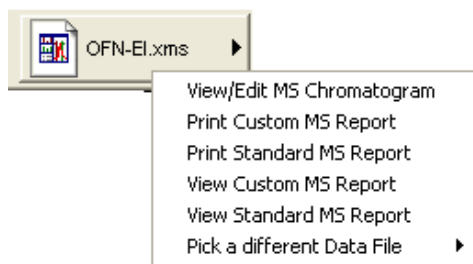
Quick Start		Run a sample without using a Sample List.
-------------	---	---

Quick Link Buttons

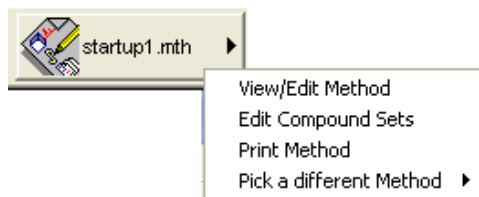
The QuickLink buttons are on the right of the application icons. They correspond to most recently used Data Files and Methods.



Most Recently Used Data File: Display options for the Most Recently Used Data File or select a different data file from the list of most recently used files.



Most Recently Used Method: Display operations that can be performed on the Most Recently Used Method or select a different method file from the list of most recently used method.



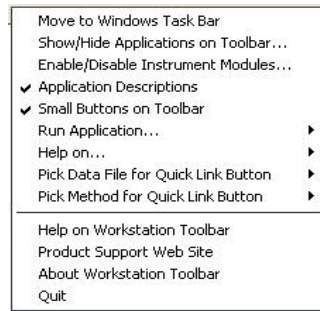
Workstation Toolbar Options

Moving the Workstation Toolbar

Move the Workstation Toolbar to any edge of the Windows screen. Click an area of the Workstation Toolbar that does not contain Application or QuickLink buttons and drag the toolbar to the preferred edge of the screen. The next time you open Workstation the toolbar will be at that spot.

Workstation Toolbar Menu

Put the cursor over an area of the Workstation Toolbar without an application or QuickLink button, and right-click to display the menu.



Move to Windows Taskbar

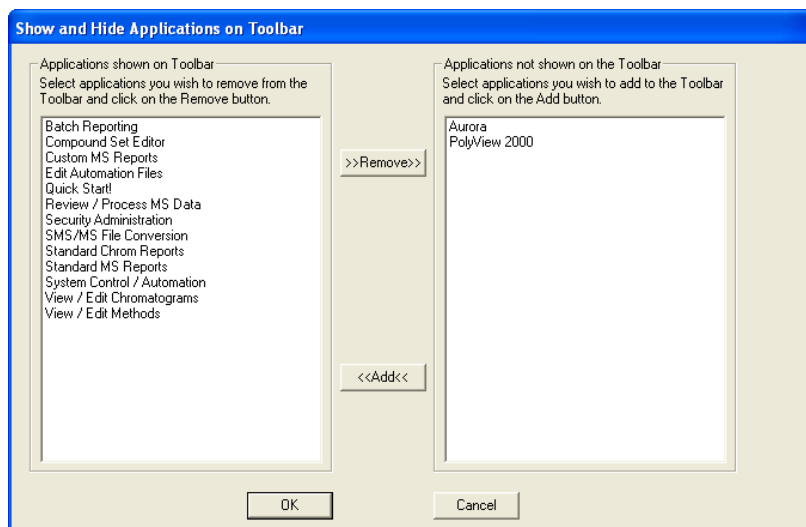
Display the Workstation Toolbar as a Windows Taskbar icon.

Click **Move to Windows Taskbar** from the **Workstation Toolbar** options menu and the Taskbar icons appear in the lower right of the Windows Taskbar. Click the **Workstation Toolbar** icon to display the options menu.

Show/Hide Applications on Toolbar

Select the applications for the Workstation Toolbar. The left side lists the applications shown on the toolbar and the right side list the applications that are installed but not shown on the toolbar.

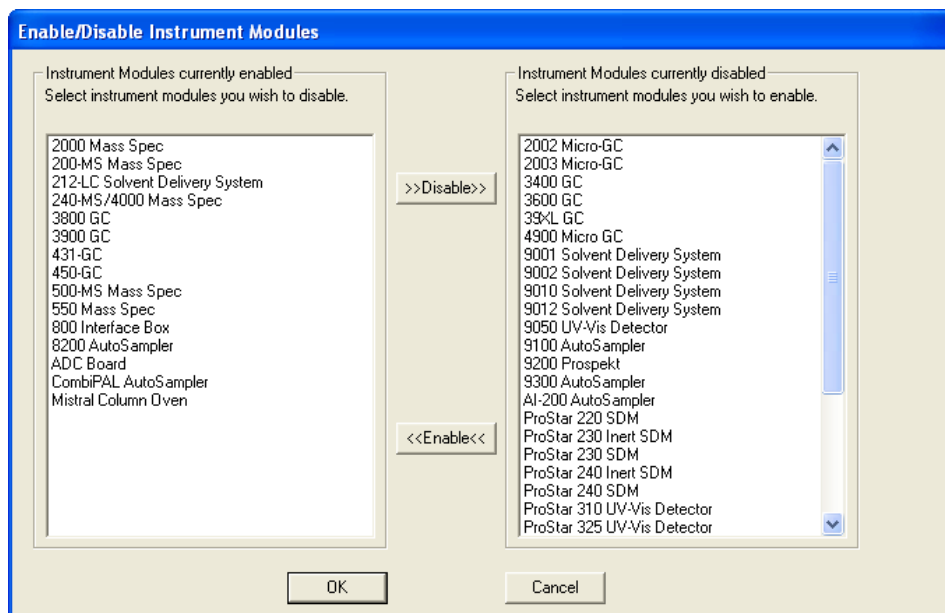
- To remove an icon from the toolbar, select it from the top list and click **Remove**.
- To add an icon to the toolbar, select it from the bottom list and click **Add**.



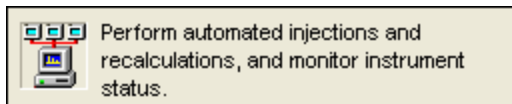
Enable/Disable Instrument Modules

Enable instrument modules. When an instrument module is available, it appears in System Control. If the corresponding instrument is connected and turned on, you can create a Method section for it, and format reports. The list on the left shows all instrument modules that are currently installed and enabled. The list on the right shows all instrument modules that are installed but not enabled.

- To disable an instrument module, select it from the list on the left and click **Disable**.
- To enable an instrument module, select it from the list on the right and click **Enable**.



Application Descriptions



When checked, a description of an application is displayed when the cursor moves over the icons.

Small Toolbar Buttons

When Small Toolbar Buttons is enabled, a smaller version of the Toolbar opens. Notice that the graphics for some icons are slightly different.



Run Application

List the applications in the Workstation Toolbar. Click to open an application.

Help on

Select an item from this list to display the online help.

Pick Data File for QuickLink

List of the eight most recently used Data Files in order of use. When you select a data file, it is displayed in the QuickLink button.

Pick Method for QuickLink

List of the eight most recently used Methods in order of use. Select one to display it in the QuickLink button.

Help on Workstation Toolbar

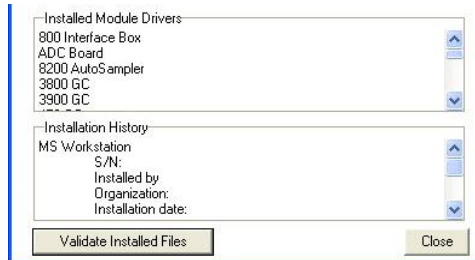
Displays help for the open application.

Product Support Web Site

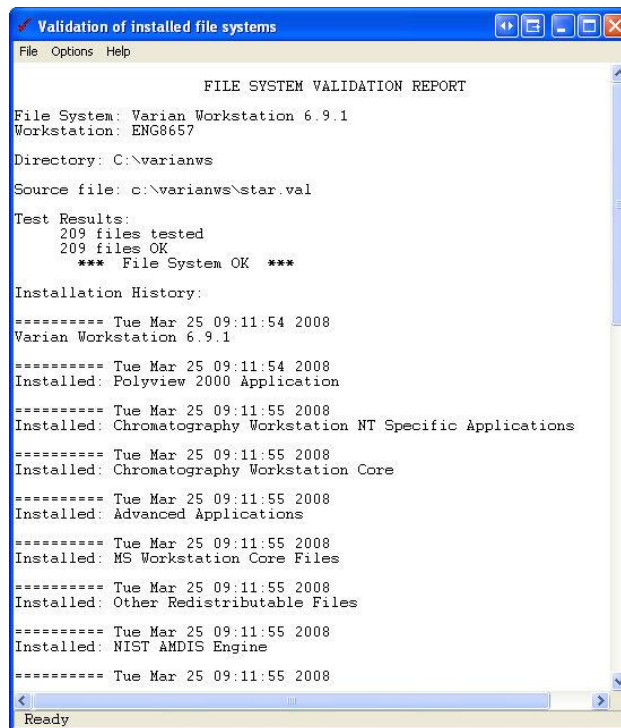
If you have Internet access and a web browser installed on your computer, click to open the MS Workstation Product Support Web Site. It has the latest software and documentation updates for the MS Workstation suite of products, and notes, tips, and answers to frequently asked questions. Visit this site periodically for new information.

About Workstation

About has information about the MS Workstation software version, installation history, and a list of the instrument modules installed. The following is an example, the software release you have may be different.



Validate Installed Files: Use checksums to test and document errors. Print a report documenting the file system tested, the results, the date printed and tested, and the ID of the person logged in (if login IDs are used). You can include a signature line. For more details, refer to online help. The following is an example



Quit

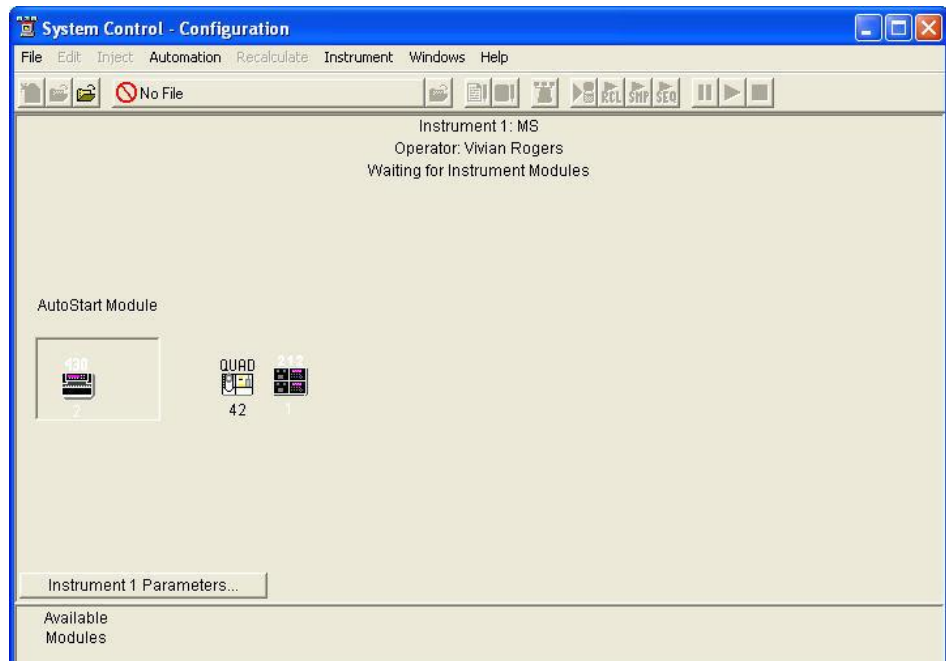
Close the Workstation Toolbar.

System Control

Overview

This section presents an overview of System Control functions. Other functions are explained in detail in later sections.

Double-click anywhere on the Configuration screen to view the Instrument Status and Control window.

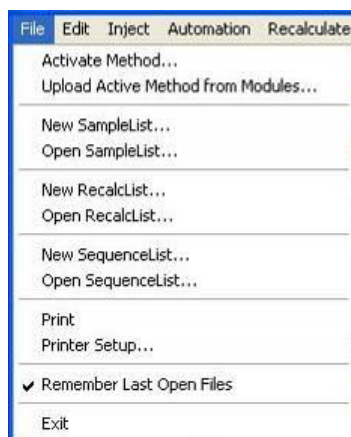


Instrument Window

Use the instrument window to monitor, the status of modules assigned to the instrument, data acquisition, inject one or more samples, and do batch recalculations. Starting at the top of the window, these features are System Control Menu, System Control Toolbar, Quad Status window, and various displays.



File Menu

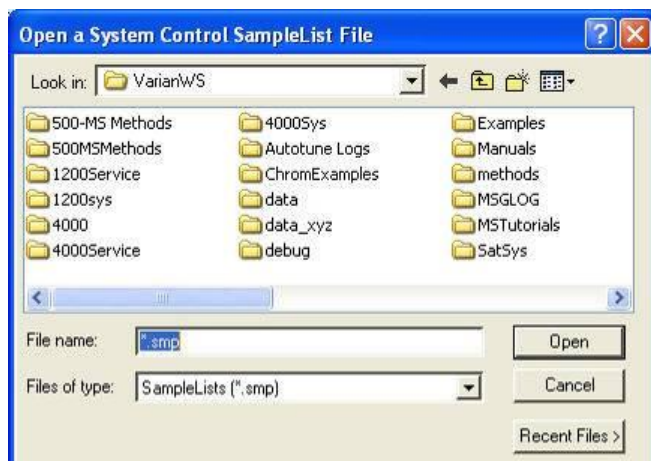


Activate Method: Select an existing method. This sets the conditions for the connected modules such as, LC, GC, MS, autosampler, and data handling.

Upload Active Method from Modules: Save conditions from the existing modules in a new or existing method. This method becomes the active method.

New SampleList: Create a SampleList.

Open SampleList: Open an existing SampleList.



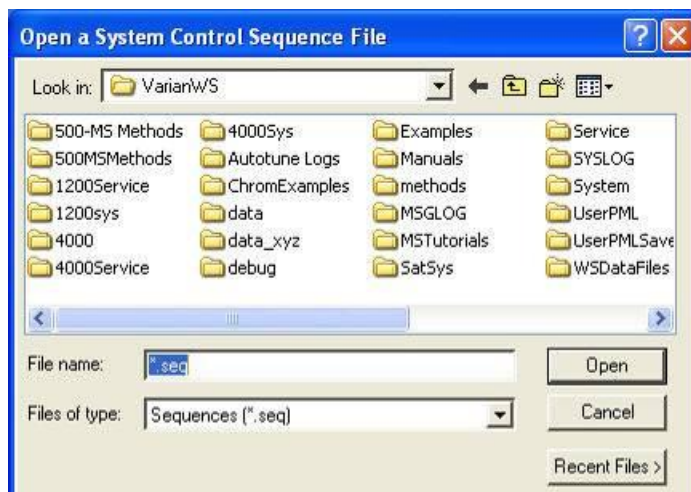
New RecalcList: Create a recalculation list.

Open RecalcList: Select an existing recalculation list.

NOTE: Process a RecalcList in System Control or in MS Data Review. In MS Data Review, from the **Quantitation** menu, select **Process/Review RecalcList**. Although Processing a RecalcList takes longer from System Control, you can use AutoLink functions including automated reporting with templates such as EnviroPro, ToxProPlus, and Multicompound Reports.

New SequenceList: Create a sequence list.

Open SequenceList: Select an existing sequence list.

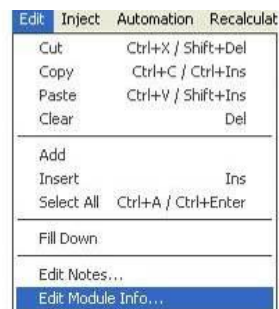


Print and **Printer Setup** are described in the MS Workstation Software Reference Manual.

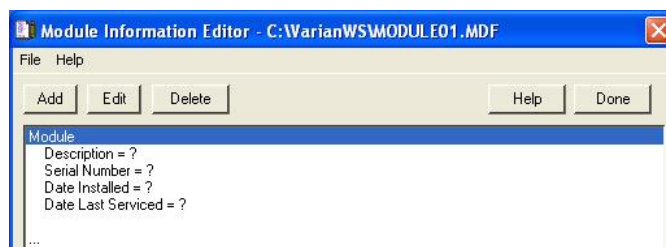
Edit Menu

Edit Module Info

Click **Edit** and select **Edit Module Info**.



Each module has a message log and a documentation screen. Use the Module Information Editor to record performance, maintenance, hours used, or other comments.



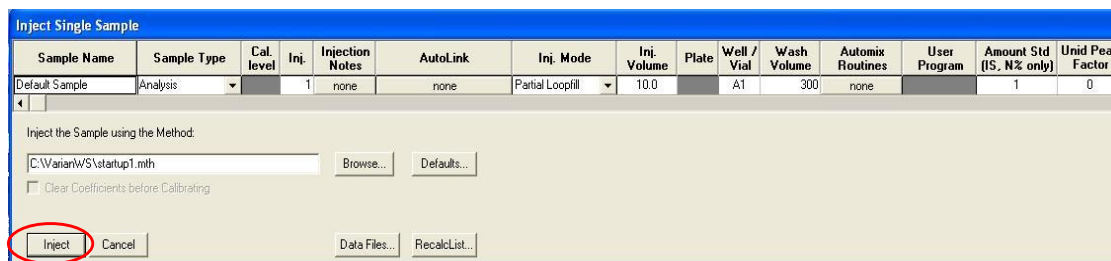
Use **Add**, **Edit**, and **Delete** to record comments.

Inject Single Sample Menu

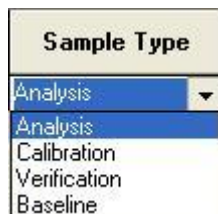
Use **Inject Single Sample** to enter sample information before making an injection. The Module window must be in acquisition mode before making an injection.



Click **Inject** in the bottom left corner to begin either a manual or an autosampler injection.



Select a **Sample Type** from the list:



Click **Injection Notes** to enter a description or comment.



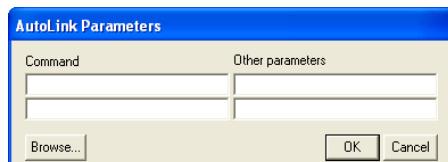
Use **AutoLink** to enter commands and parameters. Enter a command to execute a program after the data file acquisition is completed.

For more information about other fields, see the "SampleList and RecalcList Fields" Section in the *MS Data Handling User's Guide*, part number 3954038.

For example, you can activate a custom MS Report to print the sample reports.

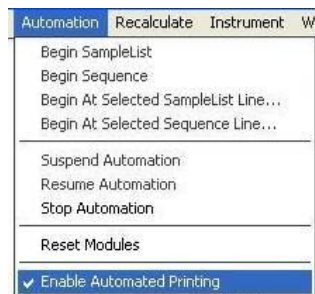
To run a Custom MS Report in automation:

1. Type the directory path and the name of the Custom MS Report template (for example C:\VarianWS\EPA525.swt). Note that Custom MS Reports templates should always be stored in the VarianWS directory.
2. Click **Browse** to select the command executable file.
3. Click **OK** entering a selection.



Automation Menu

The following shows the Automation menu and describes the options.



Begin SampleList: Automation begins at line 1 and ends at the last line. Open SampleLists from the File menu.

Begin Sequence: Begin an open SequenceList. You can change methods and SampleLists during an automated run. Open the Sequence from the File menu.

Begin At: Start automation at a particular sequence or SampleList line and run until the last line is completed. A SampleList or SequenceList must be open to use this feature.

Suspend Automation: Stop automation after the last completed sample.

Resume Automation: Start automation after it was suspended. Automation starts from where it was suspended.

Stop Automation: Stop automation immediately and reset all modules.

Reset Modules: Bring the various modules to their ready states.

Enable Automated Printing: Allow printer functions to work during automation.

Recalculate Menu

The following shows the Automation menu and describes the options.

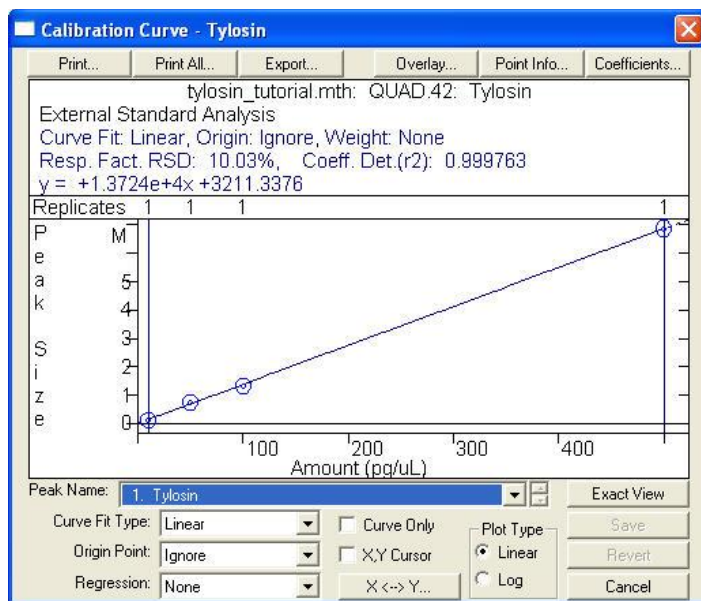


Begin RecalcList: Start an automated Recalculation. A Recalculation list must be opened under the File menu.

Begin at Selected RecalcList Line: Process a Recalculation list starting with a chosen line and proceeding with the rest of the list.

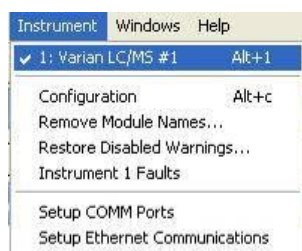
View Calibration Curves: View curves for the calibrated compounds in the active method. The Calibration Curve is saved as part of the Method.

NOTE: Recalculations can be done in System Control or in MS Data Review. From the command Quantitation, select Process/Review Recalc List. Processing a Recalc List takes more time when done from System Control than in MS Data Review but has the advantage of allowing AutoLink functions such as automated reporting with Custom MS Reports templates such as ToxProPlus or EnviroPro.



Instrument Menu

The following shows the Instrument menu and describes the options.



Varian LC/MS: The configured instrument. NOTE: Enter information in **Instrument Parameters** in the **Configuration** screen.

Configuration: Add new modules to the existing instrument.

Remove Module Names: Remove any associations between Module Names and Module Addresses. This allows you to connect a Module with a different Module Name at that address. The next time the associated Module connects at that address, you will be prompted to select the correct name for the Module.

Instrument 1 Faults: View faults in a module of in Instrument 1. Use the update key to check for new faults without opening the dialog box.



Setup Ethernet Communication: Set up communication between the 450-GC or 431-GC or other Ethernet modules and System Control.

Setup COMM Ports: Set up communication between System Control and modules communicating with the Workstation through the Serial ports on the PC. The first time you start System Control, the Star Communication Configuration Wizard starts automatically.

Windows Menu



Show Module Windows: Display the configured module windows. In this example, the modules are the 212-LC Pumps, the ProStar 430 AutoSampler, and the Quad.

Iconize Module Windows: Create icons of individual module windows at the bottom of the screen.

Show Automation Windows: View the open automation screens. The possibilities are SampleList, RecalcList, and SequenceList.

Iconize Automation Windows: Create an icon of any open automation screen windows to access windows behind the automation windows.

Arrange Icons: Arrange existing icons in a row at the bottom of the System Control window.

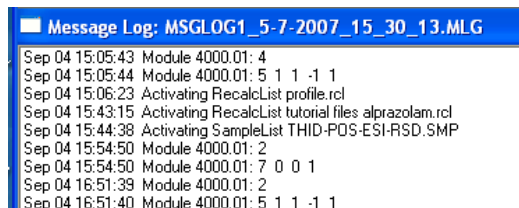
SequenceList: Display the active SequenceList.

SampleList: Display the active SampleList.

RecalcList: Display the active RecalcList.

Instrument 1 Status: View the status of the modules connected to the system.

Message Log: View the event log for the MS module. The log error messages for all configured modules.



The last section of the Windows menu displays the attached modules and their status:

- **212.24:** Stopped
- **430.33:** Ready
- **Quad.42:** Not Ready

Help Menu

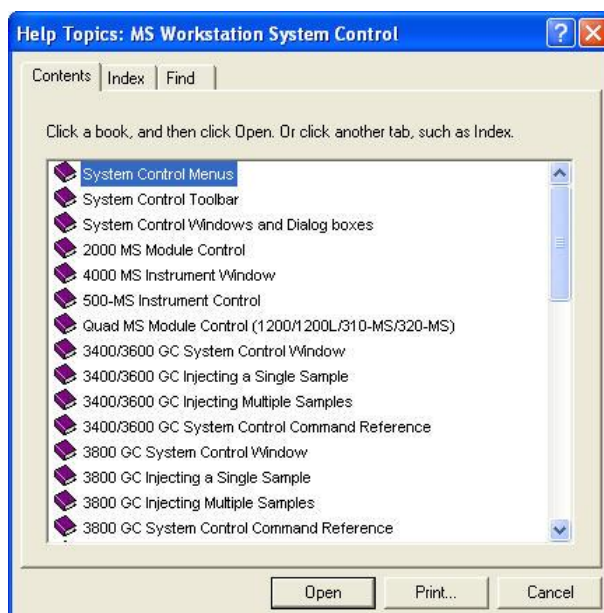
The Help menu has the following options.



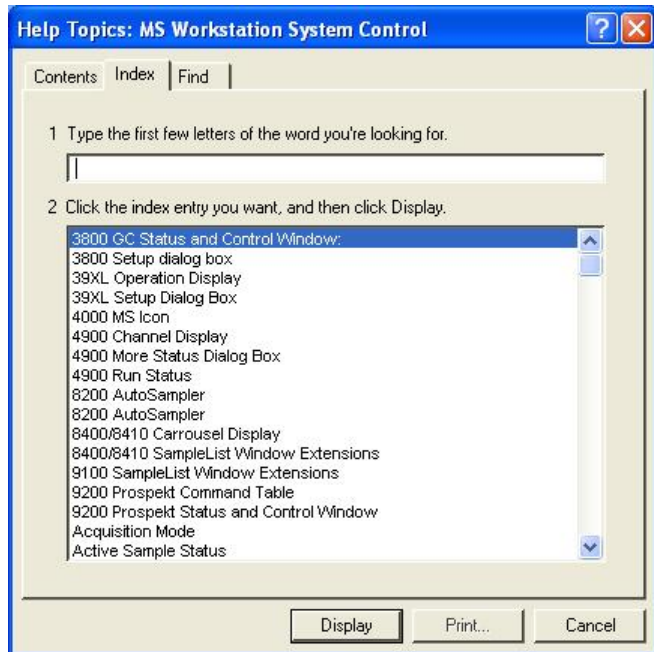
Help Topics

To find help on a topic, do the following:

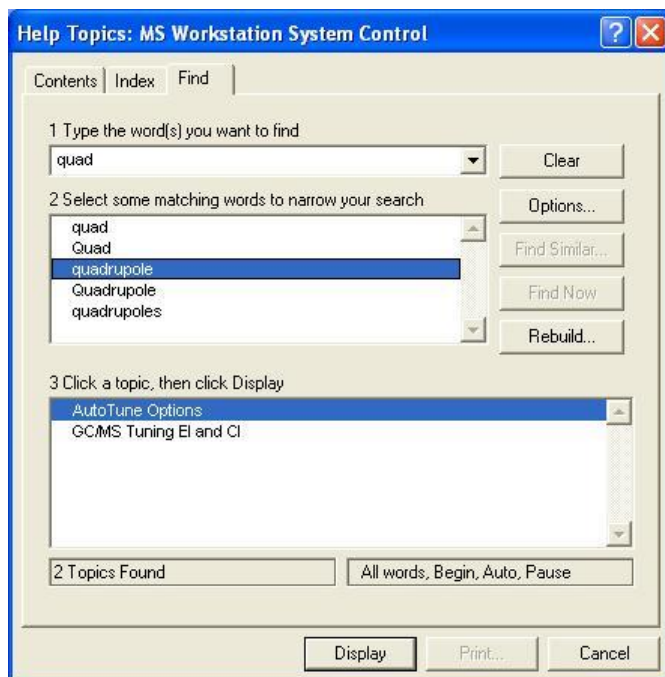
1. Select **Help Topics** to display the following. Click an item in Contents to see the online help.



2. Click the **Index** tab and enter the first few letters of a word. Click the desired selection and click **Display**.

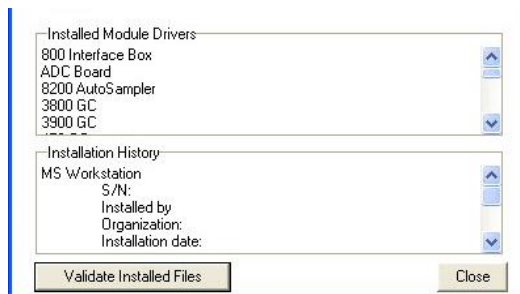


3. Enter a key word or phrase to list help topics. Click a topic and then click **Display**.



About System Control

About has information about the software version, installation information, and a list of the instrument modules installed. About System Control opens the same window as does the About Workstation Toolbar. The following is an example.



Validate Installed Files: Uses checksums to test and document errors. Print a report documenting the file system tested, the success, or failure of the test, the date printed and tested, the ID of the person logged in (if login IDs are used). You can include a signature line. For more details, refer to online help. See About Workstation on page 10.

System Control Toolbar

The system control toolbar is near the top of the screen.



The following describes the functions.

Item	Description
	Create a new automation file.
	First button: open an existing automation file.
	Second button: open the Message Log file.
	View/edit or print a Method.
	Open a Method.
	Edit notes for an automation file.
	Edit Module information for any online Module.
	Open Instrument 1 Status
	Inject a single sample.
	Start an open RecalcList.
	Start an open SampleList.
	Start an open SequenceList
	Suspend a running list.
	Begin a list.
	Stop a running list.

Quad Status and Control Window

Check the status of the instrument components, monitor data acquisition, and process data using the Quad Status and Control window. Create your preferred window configuration.

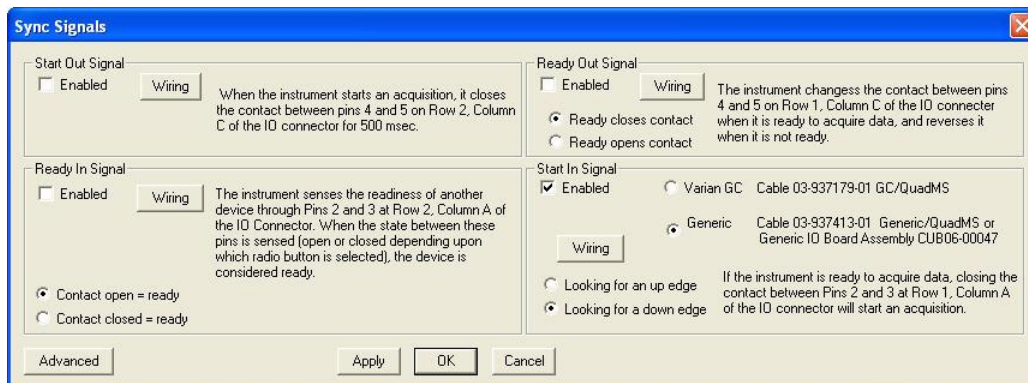
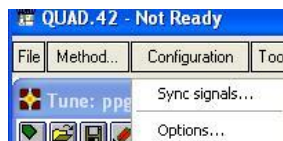


Quadrupole Module Menu

File: Open or print a file.

Method: Edit the current, active Method using Method Builder.

Configuration: Synchronization signal settings and MS Options settings.

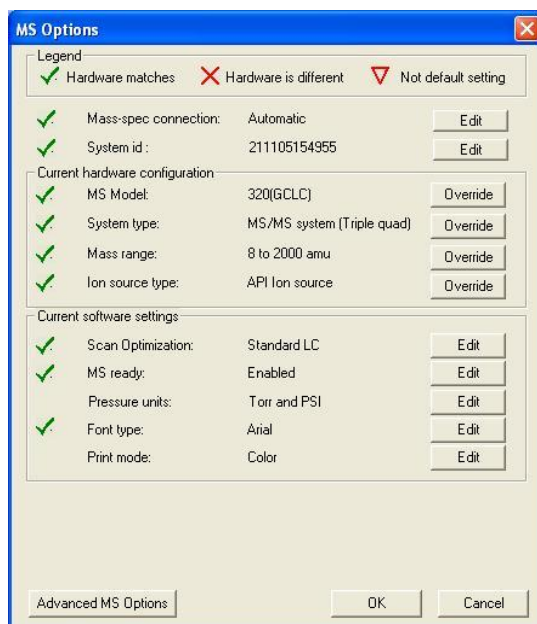


Sync Signal: Enable or disable the Start and Ready signals for external devices. To enable a Sync Signal operation, connect a cable from the device to the contact closure on the master instrument.

- Select the **Enabled** check box to activate the desired function.
- Click **Wiring** to view a wiring diagram.

MS Options: Hardware diagnostic tool. View and edit MS Options, and the current software settings.

- Check marks (✓) indicate a Hardware match
- X indicates a Hardware conflict. If an X is present, call your Varian representative.

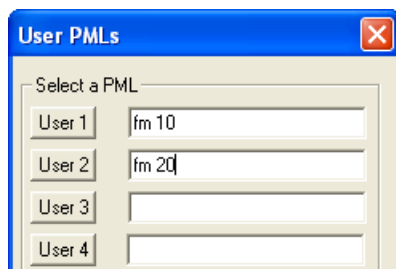


Tools: Access MS Tools such as MS/MS Breakdown, Pml Editor, Plot tic, readbacks, Bakeout system, and Overnight Standby.



Quit Macros: Stop any MS function in progress.

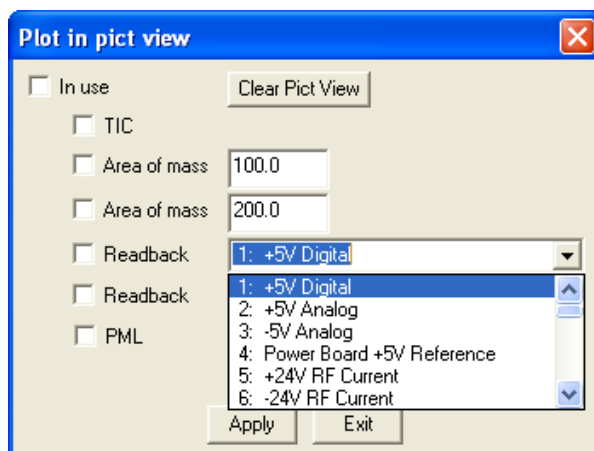
User PML: Enter up to 10 PMLs (macros written in Paw Macro Language).



Run a PML by clicking the corresponding smiley face in the toolbar.



Plot tic, readbacks: Plot a graph of the following: the TIC, the area of 2 masses, 2 readbacks, or a PML to monitor instrument status. Select the **In use** check box, the check box next to the desired parameter, and then click **Apply**.



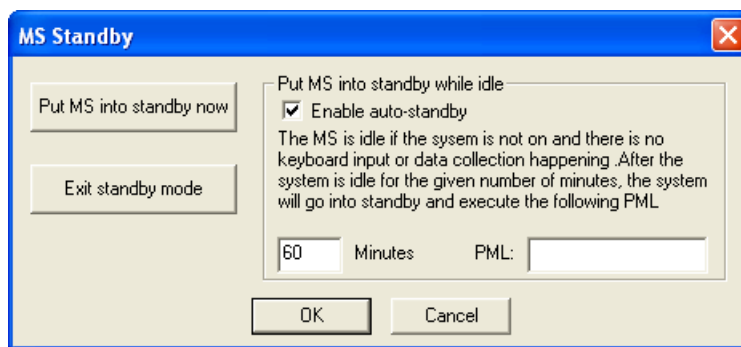
Analog output: For service use only.

MSMS Breakdown: Optimize the collision energy for any given parent mass. Used primarily for LC/MS.

Bakeout System

- GC/MS: Heat the source to 200 °C and the manifold at 50 °C for 3 hours, then cools the system to initial conditions. Also plots a graph of the source and manifold temperatures.
- LC/MS: Heat the API manifold to 65 °C and the MS manifold to 52 °C for 3 hours, and then cools the system to initial conditions. Also plots a graph of the source and manifold temperatures.

Overnight Standby: Turn off all gases and sets the MS to a low scan mass.



Troubleshooting: Run various troubleshooting procedures. See the hardware manual for more information.

Inst setup/others: Perform initial instrument setup operations.

- Coarse tune: Service use only
- Calibrate pressures: Calibrates the MS EFC/EPC pressures.

Evacuate calgas bulb: Flush calgas into the source for several minutes. Do this procedure if the calgas bulb was removed and re-installed.

Cool down and vent: Cool the source to 100 °C; then turn off the foreline pump(s) and activates a solenoid allowing air to enter the source.

Reports: Select a print view setup.

Help: Online Help and the About window.

Quadrupole Toolbar



Choose File to Display: Open and display data files, and edit headers.



Start Collecting Data: Acquire data from only the 300 Series and not other configured modules. Collect data using the current instrument conditions. Ensure that the source and detector are on before you use this feature.



Print: Print the window screen



Turn Detector On and Off: Control the filament or discharge voltage, accelerator and electron multiplier. The color of the icon indicates the following:

- Gray: Off
- Green: On
- Red: A filament is broken
- Yellow: System in process of turning on or is waiting, for example, a filament delay time. If it turns yellow and then turns gray, a fail-safe has prevented the filament and the multiplier from turning on.



Set Instrument Parameters: Set ion source and analyzer parameters, and trip points to protect the electronics and vacuum shut off. Tabbed views reflect either the GC or LC configuration.

EI/CI Source: (GC only) Turn on and off; calibration and CI gases and the filament. Set filament current, discharge voltage, and electron energy and set the Source and Transfer Line temperature.

The screenshot shows the 'Instrument Parameters' dialog box with the 'EI/CI Source' tab selected. The dialog has three tabs: 'EI/CI Source', 'Analyzer', and 'Safety'. The 'EI/CI Source' tab contains the following settings:

- Ionization mode:**
 - ☒ EI - Electron Impact Ionization
 - ☐ CI - Chemical Ionization
 - ☐ CI gas on
- Calibration Gas:**
 - ☐ On
 - ☒ Off
- Filament Current:**
 - ☐ On
 - ☒ Off ☒ In Use
 - 150 uA (50 to 500) Typical: 50
- Discharge:**
 - ☐ On
 - ☒ Off ☐ In Use
 - 1500 Volts (500 to 2000) Typical: 1500
- Electron Energy:**
 - ☐ 20 eV
 - ☒ 70 eV
 - ☐ 150 eV
- Source Temperature:**
 - Requested: 0 deg C (0 to 350) Actual: 0 °C
- Transfer Line Temperature:**
 - Requested: 0 deg C (10 to 400) Actual: 0 °C

At the bottom are buttons for 'Apply', 'OK', and 'Cancel'.

API Source: (LC Only). Select API on-off sequence, N2 filling time, and Gas pressure readbacks. Select Nebulizing gas type, and set the API Housing, Drying, and Vaporizer gas temperatures. For normal operation mode, the API on-off sequence is set to Automatic.

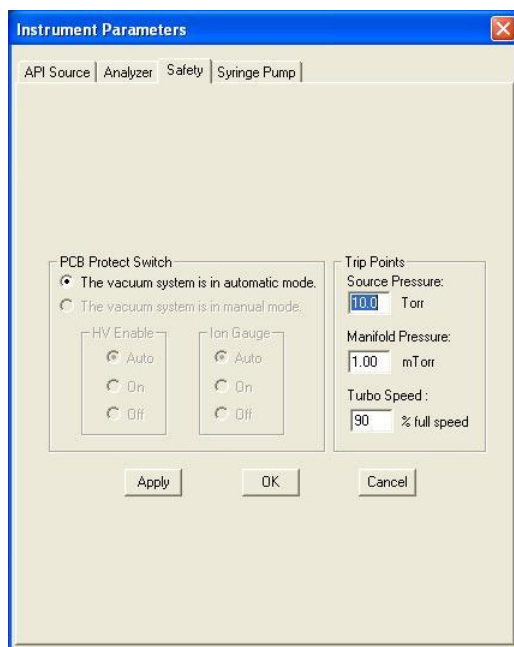
The screenshot shows the 'API Source' tab of the 'Instrument Parameters' dialog. The 'API Analyzer voltages off' section has 'API on-off sequence' set to 'Automatic'. 'N2 Filling time' is 10 Sec and 'Equilibration time' is 10 Sec. 'API Head Voltages on' is unchecked. In the 'Gases' section, 'Drying gas' is 18 psi, 'Nebulizing gas' is 70.0 psi, and 'Vortex gas' is 5.00 psi. 'Nebulizing gas type' is set to 'N2'. In the 'Heaters' section, 'API Housing (0-65)' is checked with a temperature of 50 (actual 50 °C (36% on)). 'Drying gas (50-400)' is unchecked with a temperature of 200 (actual 37 °C (0% on)). 'Vortex gas' is unchecked with a temperature of 50 (actual 38 °C (0% on)).

Analyzer: Vent the system and set the manifold temperature. Turn the CID gas on and off, set the electron multiplier (detector) voltage, and turn the Extended Dynamic Range on or off.

The screenshot shows the 'Analyzer' tab of the 'Instrument Parameters' dialog. In the 'Pumps' section, 'High Vacuum' is selected and the 'Vent' button is visible. 'Turbo Speed' is 99 %. In the 'CID gas' section, 'CID gas' is 'On' and 'CID gas pressure' is 2.00 mTorr. In the 'Detector (500 - 2000 Volts)' section, 'Off' is selected, 'Extended Dynamic Range' is unchecked, and 'Fixed' is selected with a voltage of 1500 Volts. The 'Optimize' button is visible. In the 'Manifold' section, 'Manifold temperature' is 42 Deg C (range 18 to 65, typical 40). 'Internal Air temperature' is 33 Deg and 'Manifold Pressure' is 1.3e-5 Torr. At the bottom, it states: 'Detector optimum = 1890 Volts', 'Detector calibration is recommended every 30 days', and 'Detector gain last computed Apr 10, 2007'.

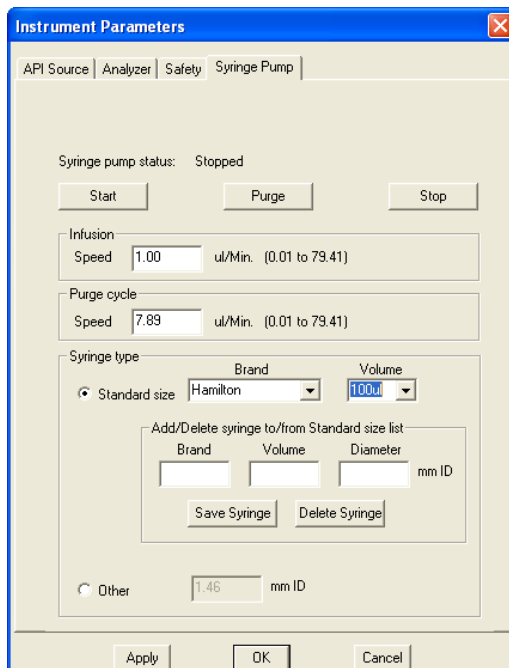
Safety: There are three sections and only Varian Representatives can change them.

- High voltage enable and Ion Gauge modes
- Trip points of the source pressure, manifold pressure and turbo speed
- Status of the PCB Protect Switch



The 'Instrument Parameters' dialog box is shown with the 'Safety' tab selected. It contains three main sections: 'PCB Protect Switch', 'HV Enable', and 'Ion Gauge'. The 'PCB Protect Switch' section has two radio buttons: 'The vacuum system is in automatic mode.' (selected) and 'The vacuum system is in manual mode.'. The 'HV Enable' and 'Ion Gauge' sections each have three radio buttons: 'Auto' (selected), 'On', and 'Off'. To the right, the 'Trip Points' section has three input fields: 'Source Pressure' (10.0 Torr), 'Manifold Pressure' (1.00 mTorr), and 'Turbo Speed' (90 % full speed). At the bottom are 'Apply', 'OK', and 'Cancel' buttons.

Syringe Pump: Only available for the 320-MS LC/MS or LC/GC/MS instruments. Refer to the Hardware manual for more information.



The 'Instrument Parameters' dialog box is shown with the 'Syringe Pump' tab selected. It displays the 'Syringe pump status' as 'Stopped' with 'Start', 'Purge', and 'Stop' buttons. Below are two sections: 'Infusion' and 'Purge cycle', each with a 'Speed' input field (1.00 and 7.89 ul/Min. respectively). The 'Syringe type' section has a 'Standard size' radio button (selected) with 'Brand' (Hamilton) and 'Volume' (100) dropdowns. Below this is a table to 'Add/Delete syringe to/from Standard size list' with columns for Brand, Volume, and Diameter (mm ID). At the bottom of this section is an 'Other' radio button with a '1.46 mm ID' input field. 'Save Syringe' and 'Delete Syringe' buttons are also present. At the very bottom are 'Apply', 'OK', and 'Cancel' buttons.



Define Scan Method: Set currently active scan parameters for Q1 and Q3, acquisition of centroid or profile data, and detection of positive or negative ions. Refer to Acquisition Method Window for more information.

	Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Req. Dwell Time	Act. Dwell Time
1	Pos.	219.00		50.00	300.00		5.000	0.120	0.166



AutoTune: Automatically tunes lenses, Q1 and Q3, and calibrates the mass scale. For information on the AutoTune process, refer to Autotune Functions and Options.

Module Views



The five default views are:

View I: Displays Quad Instrument status, Profile, Centroid, and Readbacks windows.

View II: Displays Quad Instrument status, Chromatogram, Spectra, and Centroid windows.

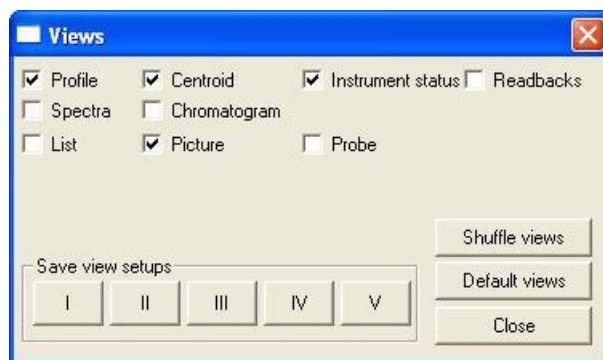
View III: Displays Quad Instrument status, Chromatogram, Spectra, and Profile windows.

View IV: Displays Quad Instrument status, Chromatogram, Spectra, and Library windows.

View V: Displays Quad Instrument status, Chromatogram, List, and Picture windows.



Select Views: Edit the five preset views. Select and display Views in the Quad window, shuffle them between different arrangements, and save them as I, II, III, IV, or V. Reset the settings with the Default button.



Profile: Real time plot of the digital signal acquired over the mass ranges scanned (profile data).

Spectra: Display acquisition of either profile or centroid spectra from the chromatograms.

List: Program for temporary storage of lists of numbers for manipulation or statistical analysis by Paw macro commands.

Centroid: Real time bar graph display of the mass peaks (centroid) of the digital signal acquired over the mass ranges scanned.

Chromatogram: Real time or post acquisition display of chromatograms.

Picture: Display program for graphing and drawing using Paw macro commands.

Instrument Status: Graphic of the analyzer, with temperatures and pressures.

Readbacks: Real time text display of either analog or digital parameters. Readbacks are a valuable resource for fast diagnostics and include voltages, temperatures, pressures, and analog and digital signal values. Monitor Readbacks are plotted in the Pict view, as a function of time other variables. You can include Readbacks a trace in a data file. Readbacks are updated about once every second.

Caution: Readback values are updated once every second whereas the RF and some DC voltages vary significantly faster during scanning or during pos/neg switching. As a result, the only meaningful readback values of these fast varying parameters are obtained when the scan is zoomed in on one mass and when there is no polarity switching.

Probe: Real time text and plot display of either the DIP or DEP probe, which is an option for either 320-MS or 300-MS systems.

AutoTune

NOTE: The Hardware manual has a detailed description of AutoTune.

AutoTune optimizes the sensitivity, resolution, and mass calibration of the instrument.

For LC/MS, a reference compound, such as polypropylene glycol (PPG) is used as a tuning solution. A custom tuning solution can also be used.

For GC/MS, FC-43 is the tuning solution. A supply bulb is inside the front panel.

Each quadrupole can be tuned in both polarities. A report with a display of peak shapes and intensities and a text report with tuning details are displayed and saved to c:\varianws\methods directory. See the following.

```
hardware diagnostics report for Varian Quadrupole Mass Sp
time: 13:45:11
no errors detected. Proceeding with autotune.

-----
tune report for Varian Quadrupole Mass Sp
time: 13:51:32  Tune file: ppg (Tuned on 13 Oct 2009)
ionization mode:ESI                      Scan Optimization: Standard GC      (EOB)

  Exact  Measured  Peak  Relative  Peak  valley  Resolution
  mass   mass     height height  width  (% of iso) (m/delta-m)
  (amu)  (amu)      (mV)  (%)      (amu @ 50%) (% of iso)
59.0    59.0      2.753 100.000  0.69  100      96
175.1   175.1   1.142 30.422   0.73  50       240
442.3   442.3   1.031 27.472   0.72  48       610
790.6   790.6   0.239 9.705    0.75  31      1053
1138.8  1138.8     0.124 1.294    0.78  29      1455
```

```
(Detector = 1800 V)
tuning of quad 1 in positive mode completed.

-----
```

```
tune report for Varian Quadrupole Mass Sp
time: 13:58:00  Tune file: ppg (Tuned on 13 Oct 2009)
ionization mode:ESI                      Scan Optimization: Standard GC      (EOB)

  Exact  Measured  Peak  Relative  Peak  valley  Resolution
  mass   mass     height height  width  (% of iso) (m/delta-m)
  (amu)  (amu)      (mV)  (%)      (amu @ 50%) (% of iso)
59.0    59.0      4.120 100.000  0.70  100      84
175.1   175.1   1.841 37.979   0.72  66       245
442.3   442.3   0.703 16.263   0.72  50       610
790.6   790.6   0.104 2.415    0.77  43      1021
1138.8  1138.8     0.052 0.738    0.85  29      1336
```

```
(Detector = 1800 V)
tuning of quad 3 in positive mode completed.

-----
```

```
tune report for Varian Quadrupole Mass Sp
time: 14:02:36  Tune file: ppg (Tuned on 13 Oct 2009)
ionization mode:ESI                      Scan Optimization: Standard GC      (EOB)

  Exact  Measured  Peak  Relative  Peak  valley  Resolution
  mass   mass     height height  width  (% of iso) (m/delta-m)
  (amu)  (amu)      (mV)  (%)      (amu @ 50%) (% of iso)
45.0    45.0      6.209 100.000  0.68  100      66
409.3   409.3   0.084 1.357   0.78  43       602
817.6   817.6   0.079 1.277   0.87  31       941
1049.7  1049.7   0.109 1.750   0.77  46      1371
```

```
(Detector = 1800 V)
tuning of quad 1 in negative mode completed.

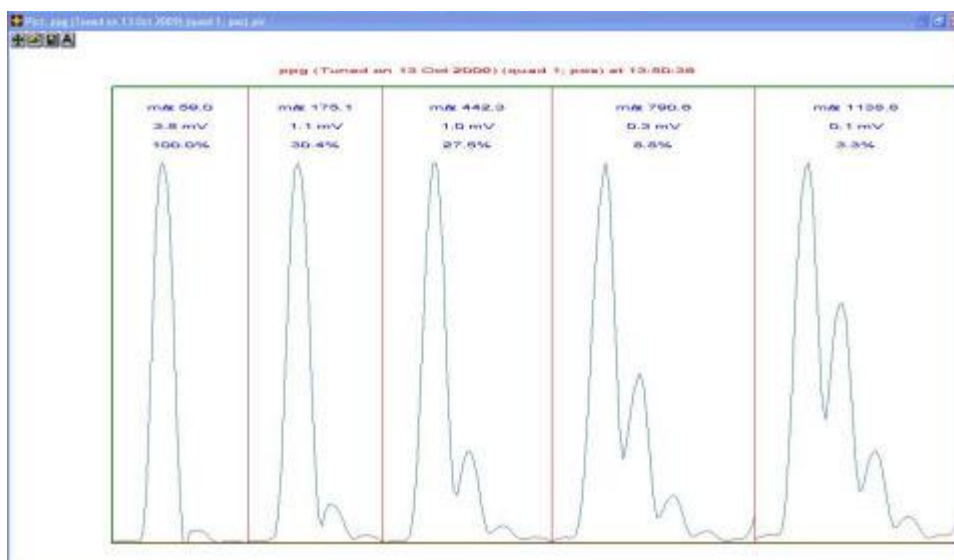
-----
```

```
tune report for Varian Quadrupole Mass Sp
time: 14:07:59  Tune file: ppg (Tuned on 13 Oct 2009)
ionization mode:ESI                      Scan Optimization: Standard GC      (EOB)

  Exact  Measured  Peak  Relative  Peak  valley  Resolution
  mass   mass     height height  width  (% of iso) (m/delta-m)
  (amu)  (amu)      (mV)  (%)      (amu @ 50%) (% of iso)
45.0    45.0      4.163 100.000  0.67  100      67
409.3   409.3   0.047 1.135   0.78  29       599
817.6   817.6   0.053 1.267   0.79  34      1031
1049.7  1049.7   0.057 1.369   0.86  33      1217
```

```
(Detector = 1800 V)
tuning of quad 3 in negative mode completed.

-----
```



Tune Stability

For optimum tune stability, the temperature of the mass analyzer must be stable and at the set point temperature of the manifold before you start AutoTune. This may take several hours if the instrument has not been under vacuum for a long time.

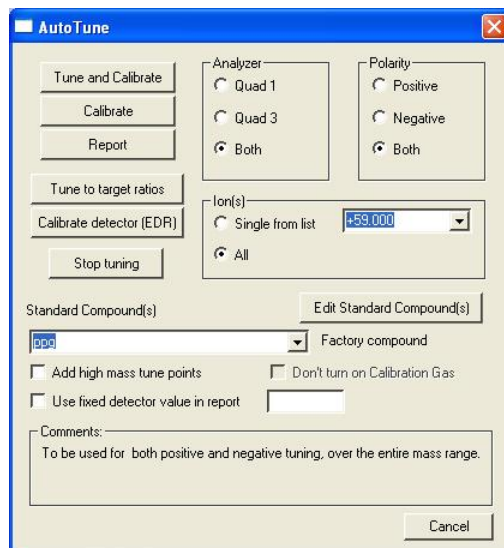
The tuning compound signal must be stable before starting AutoTune (Cal Gas on for at least 10 minutes, or PPG signal stable).

NOTE: It is not necessary to tune the instrument daily. If there is a significant loss of signal, the ion source may be contaminated. Clean the ion source and AutoTune.

Tuning is not required after changing or replacing an ion volume; however, tuning the instrument after cleaning the ion source is recommended. This optimizes the instrument and ensures that the instrument is operating properly.

AutoTune Options

Click **AutoTune**  on the Quad toolbar. Select the Analyzer and Polarity to tune and/or calibrate.



Tune and Calibrate: Complete optimization of the mass analyzer for sensitivity, resolution, and mass calibration. Set the mass resolution with a peak width of 0.7 amu at half peak height.

A report is generated with a graphic of the peak shapes and intensities (saved with mode name and date) and a text report with detailed mass accuracy and mass abundance.

Calibrate: Update the loaded tune file by re-tuning mass resolution and re-calibrating the mass. No changes are made to settings in the ion source or the non-analyzing quadrupole. A new file name and report are created and saved.

Report: Create and save a tune report. Compare with previous reports to determine if re-tuning is required. Creating a report does not change the tune file.

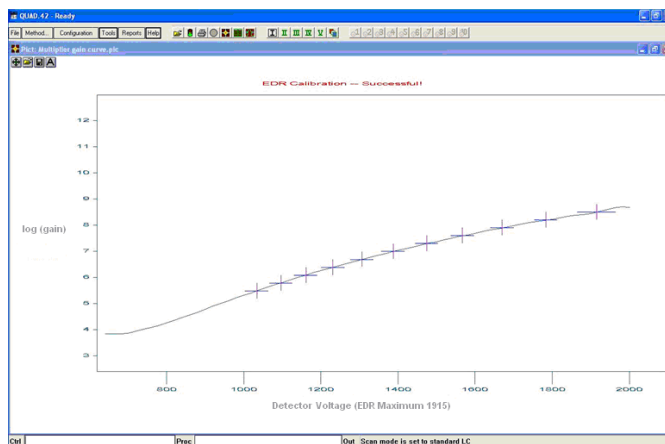
Tune to Target Ratios: Modify existing tune files. See “Tune to Target Ratios” on page 36.

Calibrate Detector (EDR): Optimize and calibrate the detector voltages over the entire dynamic range. Run this routine periodically and after replacing the detector.

The detector calibration routine has two parts.

- The first determines the optimal detector voltage for the maximum gain (EDR Maximum).
- The second calibrates the detector gain as a function of voltage for a series of gain increments. This is used to run the detector in the automatic detector adjustment mode, or Extended Dynamic Range (EDR). EDR automatically adjusts the detector voltage to accommodate either small or large ion signals over the entire dynamic range of the mass spectrometer.

The following figure shows detector gain as a function of detector voltage.



Stop Tuning: Abort the Tuning procedures and restore the most recent Tune file.

Analyzer: Tune each quad individually or tune both. Use the default (Both) setting for triple quadrupole instruments. If using a triple quadrupole as a single quadrupole, select the quadrupole in use.

Polarity: Set AutoTune polarity mode.

GC/MS

CI: AutoTune either positive or negative

EI: AutoTune positive only

LC/MS

ESI: AutoTune either positive or negative (APCI uses ESI tune file)

Ion(s): Select either a specific ion or all defined ions in the Compound list. If choosing Single from the list, select an ion from a list of ions in the Standard compound. Using a single ion adds a new data point to the loaded tune file and does not change existing points. If the same mass is present, it is tuned and changed accordingly. A report for the single mass is created and the tune file is named and saved.

Edit Standard Compound(s): Open Compound Editor and Modify a Standard compound or create a list of new compounds.

Standard Compound(s): List the Standard compounds available.

Cancel: Close AutoTune without executing a function.

Tune File Naming Conventions: AutoTune automatically names and saves each newly created tune file using the following format.

Compound Name/Mode (Date created).dac

If a file by that name already exists the file name increments.

Example: Second Negative CI Tuning on October 6th 2003

First file: FC-43 Neg CI (06 Oct 2003).dac

Second file: FC-43 Neg CI (06 Oct 2003) (2).dac

Tune to Target Ratios

Tune to Target Ratios, a GC/MS feature for EI ionization, modifies an existing mass spectrometer tune file so that relative ion ratios match user-defined target criteria. Examples are the ion ratio requirements for running EPA methods 524 (BFB) or 8270 (DFTPP) for GC/MS with an EI source.

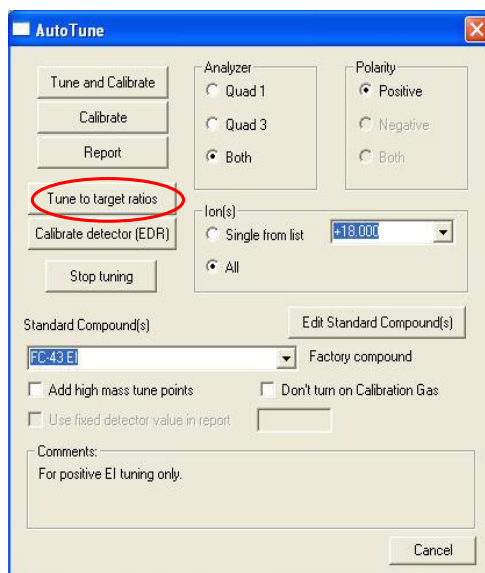
The routine adjusts the ratios relative to the base peak of 3 to 5 calibration gas ions that are relatively far apart in the mass spectrum. These ions are selected for their proximity to ions of importance in the sample spectrum. Ordinarily, this brings the entire spectrum within target ion ratio requirements. Since it is not possible to make an ion peak larger, the ratio adjustments reduce the ion peak sizes and decrease some sensitivity. Therefore, you must verify that the ion ratios in the compound of interest (usually BFB or DFTPP) are within acceptable parameters with the existing AutoTune file before running this program.

Click one of the following:

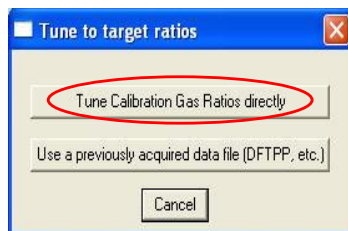
- Tune the Calibration Gas Ratios directly.
- Use a previously acquired data file.

To tune the calibration gas ratios directly:

1. Open the **AutoTune** window.
2. Click **Tune to target ratios**.



3. In the Tune to target ratios window, click **Tune Calibration Gas Ratios directly**.



4. Select the Tune Compound data file. Select a data file that has Ion ratios that normally pass DFTPP and BFB EPA 8220 requirements. If other ion ratios are required, click **Edit** in the **Tune to target ratios directly** window.
5. If editing the ion ratio list, input the ion mass in the left column and the target ratio relative to the base peak in the right column. A base peak with 100% Area must be in the list. Click **Save**.

Mass	% Area
69.0	100.0
131.0	55.0
219.0	50.0
414.0	2.0
502.0	2.0

Buttons: Save, Restore, Close

6. In the Tune to target ratios directly window, click Proceed with tune button.
7. If the ion ratios selected require peak reductions over 50%, a warning window appears before the program begins tuning. Do not reduce the ion peaks this drastically because much sensitivity is lost. If the peak reductions are less than 50%, click OK.

Mass 69, target: 100.0-100.0%, measured 100.0%. Needs reduction: 48.1%

Mass 131, target: 94.0-96.0%, measured 49.0%. Needs reduction: 0.0%

Mass 219, target: 49.0-51.0%, measured 76.7%. Needs reduction: 65.8% (Too much)!!!

Mass 414, target: 1.0-3.0%, measured 6.5%. Needs reduction: 80.0% (Too much)!!!

Mass 502, target: 1.0-3.0%, measured 7.2%. Needs reduction: 82.0% (Too much)!!!

If calibration gas ratios need too much adjustment, you may want to consider first

- Checking air/water levels
- Autotune
- Cleaning the ion source

OK to proceed?

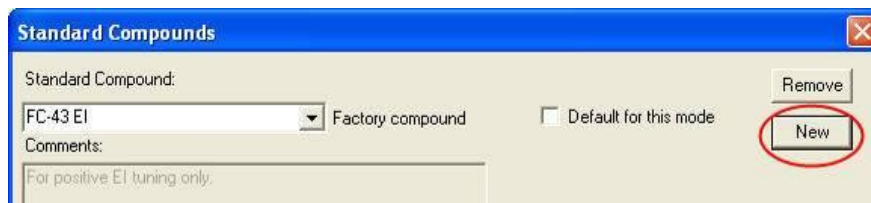
Buttons: OK, Cancel

8. After the tune completes, save the new tune file. The system does not automatically implement the new tune. To implement the new tune open the tune file using the Restore tune tables in the Instrument Status window.

Standard Compound Editor

GC/MS EI Example

1. Click **Edit Standard Compound(s)** in the AutoTune widow and the following opens.
2. Click **New** to define a new standard compound.



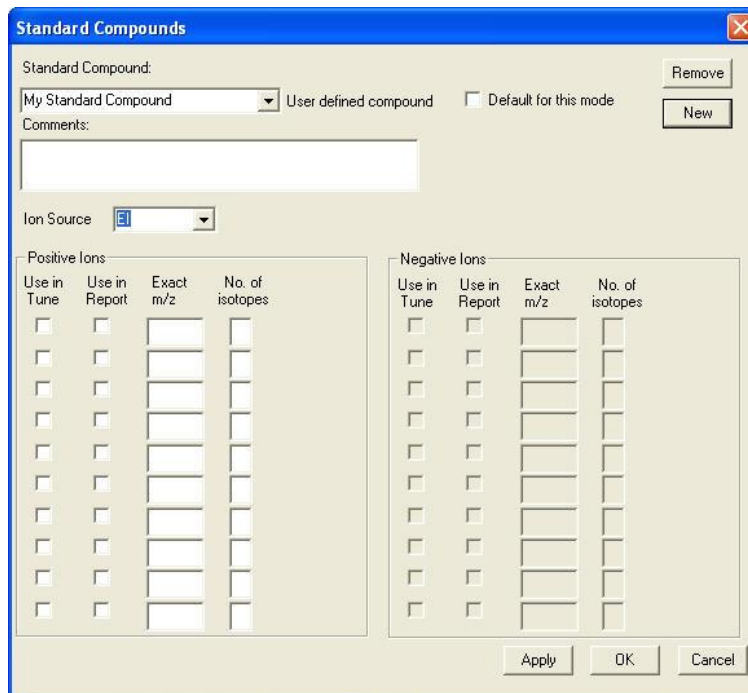
The 'Standard Compounds' dialog box is shown. It has a title bar with a close button. Inside, there's a 'Standard Compound:' label above a dropdown menu showing 'FC-43 EI'. To the right of the dropdown is the text 'Factory compound'. Further right is a checkbox labeled 'Default for this mode'. At the top right are 'Remove' and 'New' buttons. The 'New' button is circled in red. Below the dropdown is a 'Comments:' label and a text area containing the text 'For positive EI tuning only.'

3. Type a name for the new standard compound.
4. Enable the **Clear all fields** box to clear entries in the **Standard Compound** dialog box.
5. Click **OK**.



The 'Define new standard compound' dialog box is shown. It has a title bar with a close button. Inside, there's a label 'Please enter a name for the new standard compound:' above a text field containing 'My Standard Compound'. Below the text field is a checkbox labeled 'Clear all fields'. At the bottom are 'OK' and 'Cancel' buttons.

6. In the **Standard Compounds** dialog box, enter the information.



The 'Standard Compounds' dialog box is shown with more options. The 'Standard Compound:' dropdown now shows 'My Standard Compound' and the text next to it is 'User defined compound'. The 'Default for this mode' checkbox is still present. The 'New' button is still there. Below the 'Comments:' text area is an 'Ion Source' dropdown menu showing 'EI'. Below the 'Ion Source' are two tables: 'Positive Ions' and 'Negative Ions'. Each table has four columns: 'Use in Tune', 'Use in Report', 'Exact m/z', and 'No. of isotopes'. Each column has a checkbox and a text field. At the bottom are 'Apply', 'OK', and 'Cancel' buttons.

Positive Ions				Negative Ions			
Use in Tune	Use in Report	Exact m/z	No. of isotopes	Use in Tune	Use in Report	Exact m/z	No. of isotopes
☐	☐			☐	☐		
☐	☐			☐	☐		
☐	☐			☐	☐		
☐	☐			☐	☐		
☐	☐			☐	☐		
☐	☐			☐	☐		
☐	☐			☐	☐		
☐	☐			☐	☐		
☐	☐			☐	☐		

Standard Compound: List Standard Compounds for the selected mode.

Default for this Mode: Set displayed Standard Compound as the default.

New: Add a new list of Standard Compounds.

Remove: Remove a Standard Compound.

Comments: Enter information about the Standard Compound.

Ion Source: Select the ion source (EI, CI, ESI, or APCI).

Use in Tune: Select which ions to use for Tune or Calibrate. These ions are optimized.

Use in Report: Select ions for the tune report. Only the selected ions are reported.

Exact m/z: Enter the exact m/z of each ion in the Standard compound.

No. of Isotopes: Enter the number of isotopes for the ion in the tune report.

LC/MS ESI Example

1. In the AutoTune window, select **ppg** from the Standard Compound(s) list.
2. Click **Edit Standard Compound(s)**

Standard Compounds

Standard Compound: **ppg** Factory compound ☒ Default for this mode

Comments: To be used for both positive and negative tuning, over the entire mass range.

Ion Source: **ESI** ☒ Set Capillary

Positive Ions				
Use in Tune	Use in Report	Exact m/z	No. of isotopes	Capillary (Volts)
☒	☒	59.000	1	100.00
☒	☒	175.100	1	100.00
☒	☒	442.300	2	30.00
☒	☒	790.600	3	80.00
☒	☒	1138.80	3	100.00
☐	☐			
☐	☐			
☐	☐			
☐	☐			
☐	☐			

Negative Ions				
Use in Tune	Use in Report	Exact m/z	No. of isotopes	Capillary (Volts)
☒	☒	45.000	1	-40.00
☒	☒	469.300	2	-40.00
☒	☒	817.600	3	-60.00
☒	☒	1049.70	3	-80.00
☐	☐			
☐	☐			
☐	☐			
☐	☐			
☐	☐			
☐	☐			

Set Capillary (LC/MS mode only): For standard compounds that you create, if the box is checked, set the capillary voltage for each ion to the value in Capillary (volts) field. If not checked or blank, the voltage from the capillary tune table is used.

Capillary (Volts) (LC/MS mode only): If the Set Capillary box is checked, you can set the capillary voltage to be used for each tune ion, otherwise this option is not available.

If tuning with PPG, select Set Capillary and use the default capillary voltage values.

Method Builder

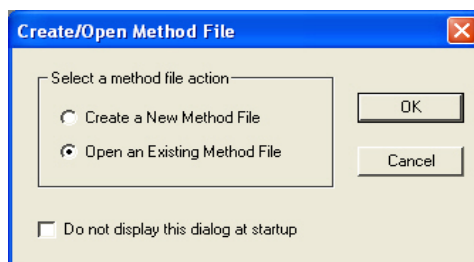
Using Method Builder

Click **Method Builder** in the MS WorkStation Toolbar.

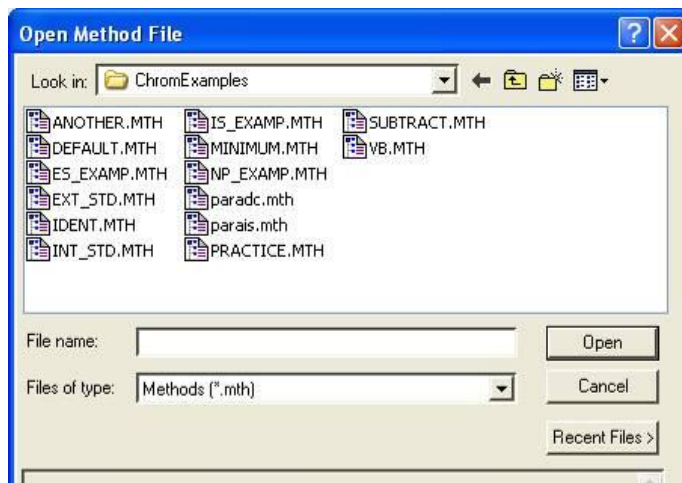


Edit an Existing Method

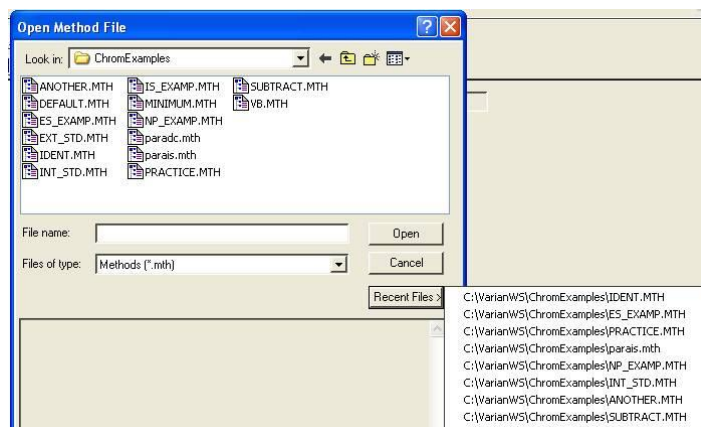
1. Click **Open an Existing Method File** and then click **OK**.



2. Select the method by doing one of the following:
 - Select the folder and then the file name.

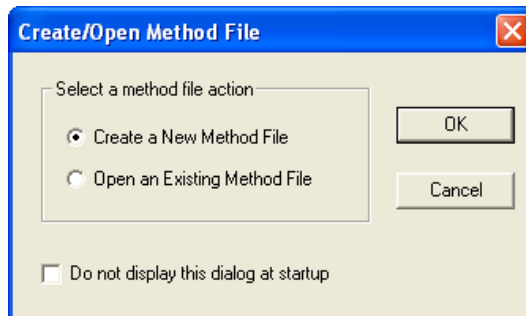


- Click **Recent Files** to display them and select one.

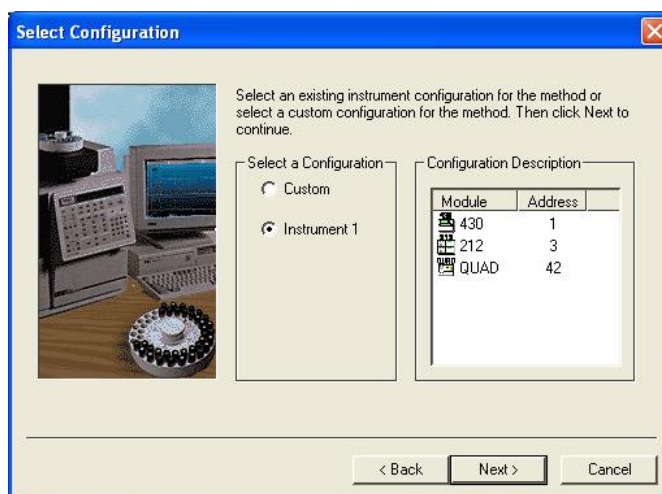


Build a New Method

1. Click **Create a New Method File** and click **OK** to open the Method Builder Wizard.

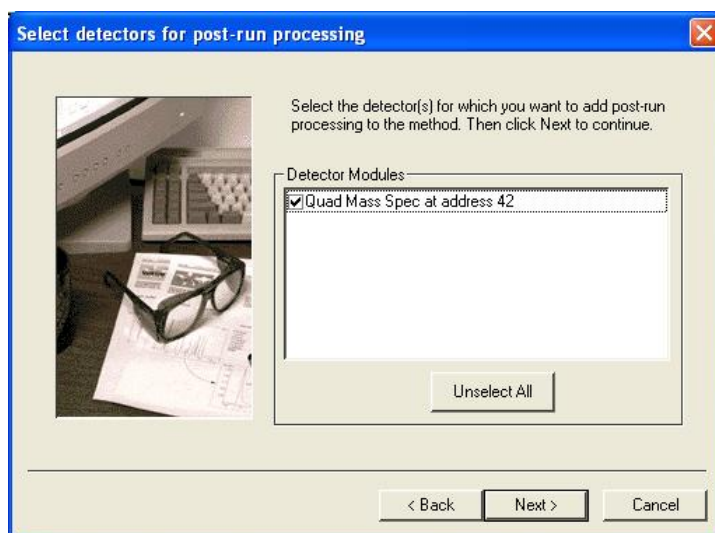


2. Select **Instrument 1**. The configured instrument is added to the method.
3. Click **Next**.



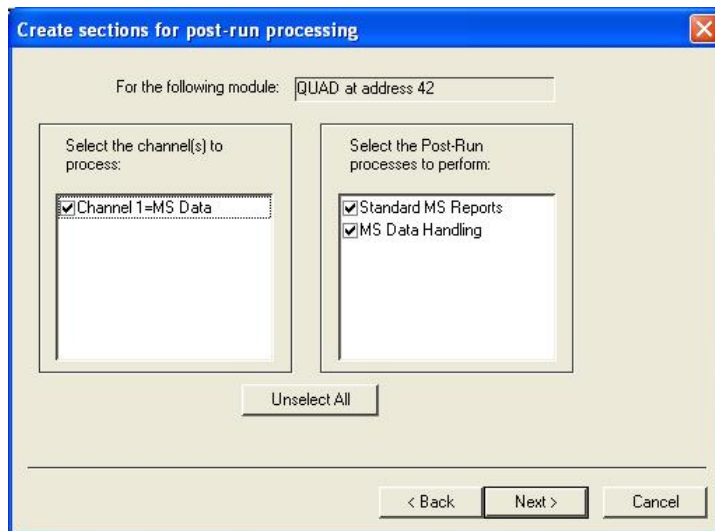
4. Select a detector. After the data is acquired, you can add data processing information to the method.

5. Click **Next**.



6. Create sections for **post-run processing**. Add MS Data Handling to enter integration, peak names, and other parameters. Add Standard MS Reports to use the standard reports.

7. Click **Next**.

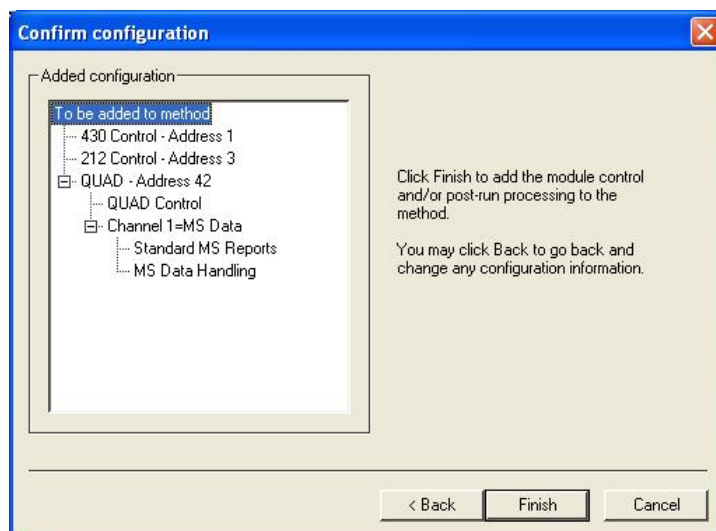


8. Review the information on the **Confirm configuration** screen.

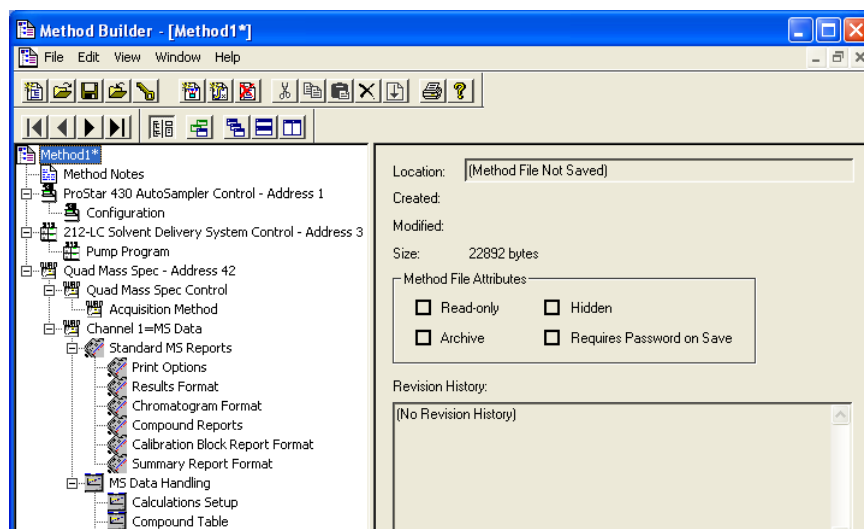
9. Click **Next**.

10. Review the configuration

- Click **Back** to make changes
- Click **Finish** to confirm.

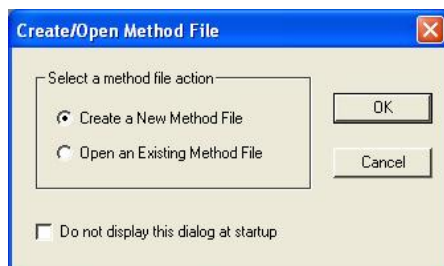


11. The new method is displayed with a navigation tree on the left side and the method workspace on the right. Click a tree entry to open that method section.

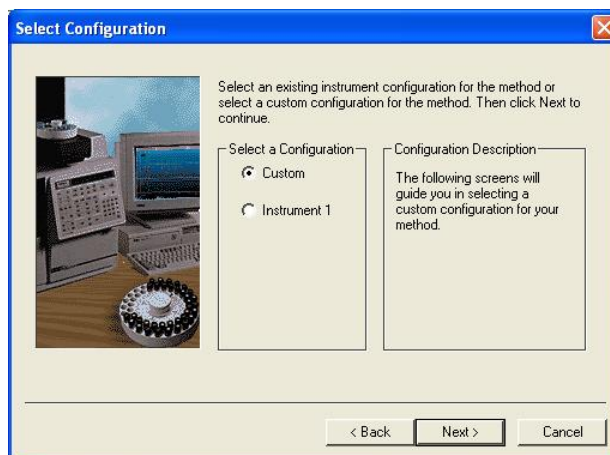


Add a Varian Instrument to a Method

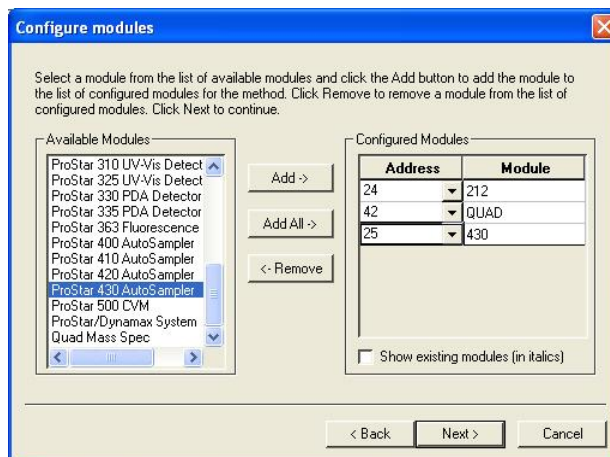
1. Select **Create a New Method File** and click **OK**.



2. Click **Custom** and then click **Next**.



3. Select an available module from the list and click **Add** to make it one of the Configured Modules. Other options are **Add**, **Add All**, or **Remove**.
4. Click **Next**.



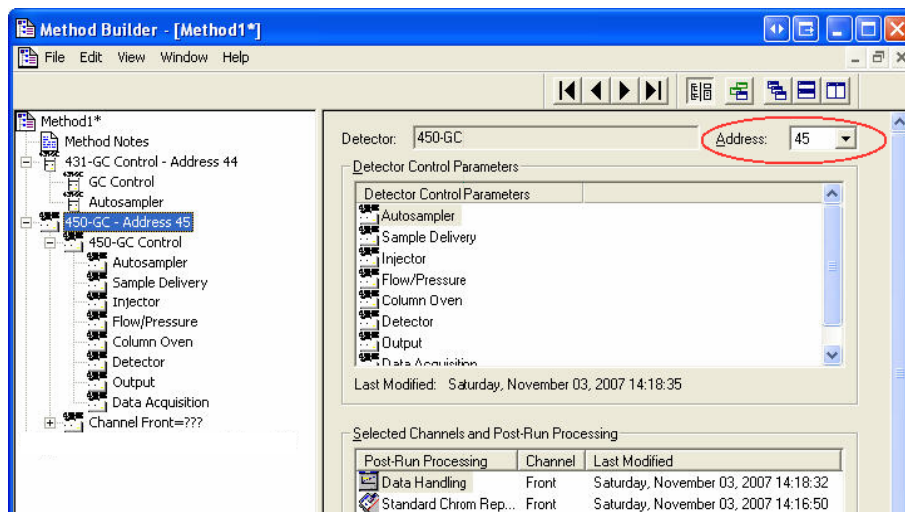
5. Continue with step 3 of "Build a New Method" on page 41.

450-GC Methods

450-GC Windows

Click **450-GC** in the Method Builder to display the Module Control Parameters.

By changing the module address in the parameter window, a method developed for an instrument using one module address can be easily modified for an instrument at a different module address.



The 450-GC Method section has eight windows:

- Autosampler
- Sample Delivery
- Injector
- Flow/Pressure
- Column Oven
- Detector
- Output
- Data Acquisition

Each window has parameters for controlling the GC during a chromatographic run. If the 300 Series MS is the only detector and the samples are injected by syringe, the Sample Delivery, Detector, Output, and Data Acquisition sections do not apply. For information on those sections, see the 450-GC User Manual.

Checking Method End Times

Editing windows, except for the Column Oven window and Detector window display the current end time of the column oven program at the bottom.

Front EFC | Middle EFC | Rear EFC |

Front EFC Type: Type 21 (for any Injector Type)

	Pressure (psi)	Rate (psi/min)	Hold (min)	Total (min)
1	10.0		20.00	20.00
2				
3				
4				
5				
6				
7				
8				

Constant Column Flow Mode
Constant Flow: ☒ Off ☐ On

Column Oven End Time: 20.00 min

If you enter program end times for parameters other than the column oven that exceed the column oven end time, the following warning is displayed.

Method Editor

The following components have program end times that exceed the Column Oven EndTime: Front EFC Type 21 Ramp; The Column Oven EndTime determines the Method EndTime on the 450-GC. Do you want to save this Method even though this condition exists?

Yes No

When the Method is downloaded to the GC, component program end times exceeding the column oven end time are truncated.

Injector Window

The Injector window contains up to three Injector Programs (Front, Middle, and Rear). The isothermal 1177 and temperature programmable 1079 injectors can be used with the 300 Series MS. Use Injector Programs to specify the temperature set point and split ratio of the isothermal 1177 Injectors, and to specify the temperature ramp and split ratio of the programmable 1079 Injector.

1079 Injector

To control the Oven Power and the Injector Coolant from the Injector window, do the following:

1. After turning the coolant and oven on, select the desired temperature in the Enable Coolant at (C) drop down list, and select the desired Coolant Timeout (min).
2. Type in a temperature ramp program to heat and/or cool the 1079 injector.
3. The first row contains the initial temperature and hold time for the 1079 injector. The 1079 equilibrates to this setting when the method is activated, and is restored to this setting after each chromatographic run is completed.
4. The following rows are for each ramp segment. Each segment ramps to the specified temperature at the specified rate (assuming the rate is achievable), and then holds the temperature for the specified time.

NOTE: The Rate field in the first row is always blank and cannot be edited. Also, the Total field cannot be edited.

Front Injector | Middle Injector | Rear Injector

Front Injector Type: 1079 Injector Oven: ☒ On ☐ Off

Injector Coolant: ☒ On ☐ Off

Enable Coolant at (C): 250.0

Coolant Timeout (min): 20.00 Split Ratio...

	Temp (C)	Rate (C/min)	Hold (min)	Total (min)
1	50.0		20.00	20.00
2				
3				
4				
5				

Add
Insert
Delete

1079 Split Ratio

If the 1079 Injector is connected to a Type 21 EFC, click **Split Ratio** to open the Split Ratio Time Program.

Front Injector | Middle Injector | Rear Injector

Front Injector Type: 1079 Injector Oven: ☒ On ☐ Off

Injector Coolant: ☐ On ☒ Off

Enable Coolant at (C): 250.0

Coolant Timeout (min): 20.00 Split Ratio...

Temp	Time	Split State	Split Ratio
1			
2			
3			
4			
5			

Split Ratio for Front 1079 + Front Type 21 EFC

Column Oven End Time: 20.00 min

Save Cancel

NOTE: The Type 21 EFC must be configured in the corresponding position in the Flow/Pressure Section before the Split Ratio can be programmed. Specifically, to build a 1079 Split Ratio Program, a Front 1079 must have a corresponding Front Type 21 EFC, a Middle 1079 must have a corresponding Middle Type 21 EFC, and a Rear 1079 must have a corresponding Rear Type 21 EFC.

Use the Split Ratio spreadsheet to build a Split Ratio Time Program to control the 1079 injector / Type 21 EFC combination.

The first row of the spreadsheet contains the Initial Split State and Split Ratio for the 1079 injector. The 1079 equilibrates to this setting when the method is activated, and is restored to this setting when each chromatographic run is completed.

The following rows contain the time-programmed settings for the 1079 Split Ratio. The Split Valve is switched to the ratio in each row at the indicated time.

This is a typical program for a splitless injection. A low split ratio conserves carrier gas while keeping contaminants from building up in the injector. The injector is kept splitless for about 1 minute so all of the analytes are focused on the column.

Use a split ratio of 100 after injection to flush residual solvent from the injector.

	Time	Split State	Split Ratio
1	Initial	On	20
2	0.01	Off	Off
3	1.00	On	100
4			
5			
6			

Column Oven End Time: 20.00 min

Save Cancel

1177 Injector

The 1177 Injector window has controls for the Injector Oven and the Split Ratio.

Front Injector | Middle Injector | Rear Injector

Front Injector Type: 1177 Injector Oven: ☒ On ☐ Off

Temperature (C): 50.0

Split Ratio...

Column Oven End Time: 20.00 min

NOTE: The EFC type in the corresponding position in the Flow/Pressure Section must be configured before the Split Ratio can be programmed. Specifically, to build an 1177 Split Ratio Program, a Front 1177 must have a corresponding Front Type 21 EFC, a Middle 1177 must have a corresponding Middle Type 21 EFC, and a Rear 1177 must have a corresponding Rear Type 21 EFC.

Use the Split Ratio spreadsheet to build a Split Ratio time program to control the 1177 injector / Type 21 EFC combination.

The first row of the spreadsheet contains the Initial Split State and Split Ratio for the 1177 injector. The 1177 equilibrates to this setting when the method is activated, and is restored to this setting when each chromatographic run is completed.

The following rows contain the time programmed settings for the 1177 Split Ratio. The Split Valve is switched to the ratio in each row at the indicated time.

The following is a typical program for a splitless injection. A low Split Ratio conserves carrier gas while keeping contaminants from building up in the injector. The injector is kept splitless for about 1 minute so that all analytes injected can focus on the column. A Split Ratio of 100 after injection flushes residual solvent from the injector.

Split Ratio for Front 1177 + Front Type 21 EFC

	Time	Split State	Split Ratio
1	Initial	On	20
2	0.01	Off	Off
3	1.00	On	100
4			
5			
6			

Column Oven End Time: 20.00 min

Save Cancel

Add
Insert
Delete
Sort

Flow/Pressure Window

The Flow/Pressure window can have up to three Electronic Flow Control (EFC) Programs (Front, Middle, and Rear).

To set up an EFC, do the following:

1. Use the tabs to select the front, middle, or rear EFC Program to edit.
2. Select the type of EFC at each position, or none if no EFC is installed at that position.

Front EFC | Middle EFC | Rear EFC

Front EFC Type: Type 21 (for any Injector Type)

	Pressure (psi)	Rate (psi/min)	Hold (min)	Total (min)
1	10.0		20.00	20.00
2				
3				
4				
5				
6				
7				
8				

Constant Column Flow Mode
Constant Flow: ☒ Off ☐ On

Column Oven End Time: 20.00 min

Add
Insert
Delete

Type 21 EFC (for 1079/1177 Injectors)

The Flow/Pressure window for a Type 21 EFC has a pressure ramp.

The first row of the spreadsheet contains the Initial pressure and hold time. After the method is activated, the EFC equilibrates to this setting, and after each chromatographic run is completed, is restored to this setting,

The following rows contain the programmed settings for each ramp segment. Each segment ramps to the specified pressure at the specified rate (assuming the rate is achievable), and then holds the pressure for the specified time.

NOTE: The Rate field in the first row is always blank and cannot be edited. Also, the Total field cannot be edited.

Front EFC | Middle EFC | Rear EFC |

Front EFC Type: Type 21 (for any Injector Type) ▼

	Pressure (psi)	Rate (psi/min)	Hold (min)	Total (min)
1	10.0		1.00	1.00
2	20.0	2.0	14.00	20.00
3				
4				
5				
6				
7				
8				

Add
Insert
Delete

Constant Column Flow Mode
Constant Flow: ☒ Off ☐ On

Column Oven End Time: 20.00 min

Enabling Constant Column Flow mode disables the spreadsheet and enables the Constant Flow rate field.

Front EFC | Middle EFC | Rear EFC |

Front EFC Type: Type 21 (for any Injector Type) ▼

	Pressure (psi)	Rate (psi/min)	Hold (min)	Total (min)
1				
2				
3				
4				
5				
6				
7				
8				

Add
Insert
Delete

Constant Column Flow Mode
Constant Flow: ☐ Off ☒ On

Pressure Pulse: ☒ No ☐ Yes

Column Flow (ml/min): 5.0

Pulse Pressure (psi): 10.0

Pulse Duration (min): 0.25

Column Oven End Time: 20.00 min

When the method is activated in System Control, MS Workstation downloads the appropriate pressure program corresponding to the Column Temperature program, the Column Setup Length and Diameter, the Carrier Gas, and the ambient Barometric Pressure. These parameters are specified on the 450-GC front panel, and the Barometric Pressure is measured by the 450-GC when the Method is downloaded. The 450-GC runs the pressure program to hold the Column Flow at the specified value as the Column Temperature is ramped during each run.

Column Oven Window

Use the Column Oven Program to specify the Coolant Parameters and Stabilization Time of the Column Oven, and to specify a programmable temperature ramp.

Turn the Coolant or the Oven on or off. Set the Coolant temperature and Coolant Timeout in minutes.

Create temperature ramp program to heat and/or cool the Column Oven.

The first row of the spreadsheet has the Initial temperature and hold time for the Column Oven. When the method is activated, the Column Oven equilibrates to this setting, and stabilizes for the specified Stabilization Time. After each chromatographic run is completed, the temperature is restored to this setting.

The following rows contain the programmed settings for each of the ramp segments. Each segment ramps to the specified temperature at the specified rate (assuming the rate is achievable), and then holds the temperature for the specified time.

NOTE: The Rate field in the first row is always blank and cannot be edited. Also, the Total field cannot be edited.

Column Oven Coolant: ☐ On ☒ Off

Enable Coolant at (C):

Coolant Timeout (min):

Stabilization Time (min):

Column Oven: ☐ On ☒ Off

	Temp (C)	Rate (C/min)	Hold (min)	Total (min)
1	50.0		2.00	2.00
2	200.0	20.0	10.50	20.00
3				
4				
5				
6				
7				
8				

Add
Insert
Delete

AutoSampler Window

The AutoSampler window has parameters for the 8400/8410 AutoSampler. The parameters include the sampling syringe size, the penetration depth for sample and solvent wash vials, the default clean and clean modes, and the injection modes.

Default clean steps are used if automation is stopped or a serious fault is detected. Select Pre and Post injection syringe clean modes.

Autosampler:

Syringe Size (uL):

Sample Depth (%):

Injection Mode:

Solvent Depth (%):

Default Clean

Vial:

Volume (uL):

Strokes:

Speed (uL/sec):

Clean Mode

Pre-Inj Solvent Flushes:

Pre-Inj Sample Flushes:

Post-Inj Solvent Flushes:

Clean Solvent Source:

Internal Standard

Use:

Vial:

Volume (uL):

Drawup Speed (uL/sec):

Pause Time (sec):

Air Gap:

More User Defined...

User Defined Parameter Sets

Manage...

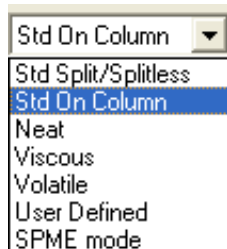
Use Prep Ahead:

Prep Ahead Delay (min):

Column Oven End Time: 20.00 min

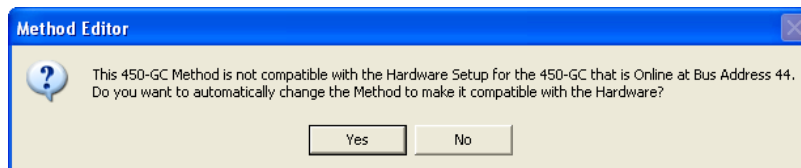
Injection Mode

There are seven injection modes: Standard Split/Splitless, Standard On-Column, Neat, Viscous and Volatile, User Defined, and SPME. See Help for a detailed description of all Injection Mode parameters.



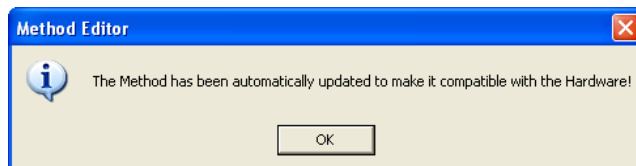
Auto-Configuring the Method

Although you edit a 450-GC Method while the corresponding GC is online in System Control, you are warned if the Method configuration does not match the hardware on the GC.



- Click **Yes** to change the Method to match the GC.
- Click **No** to accept the Method.

If you auto-configure the Method, the following dialog is displayed.

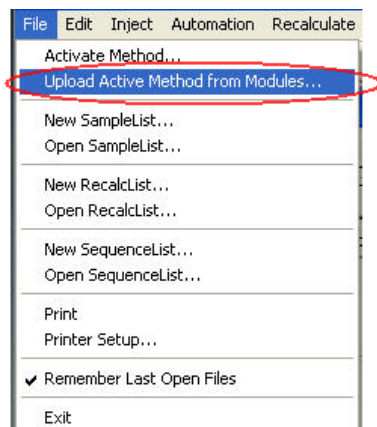


Uploading the Method from the 450-GC

Uploading the method from the GC and saving it in MS Workstation allows you to edit the local Method on the 450-GC front panel and save it on the Workstation.

To upload the 450-GC Method to System Control, click **Upload Active Method from Modules** from the **File** menu.

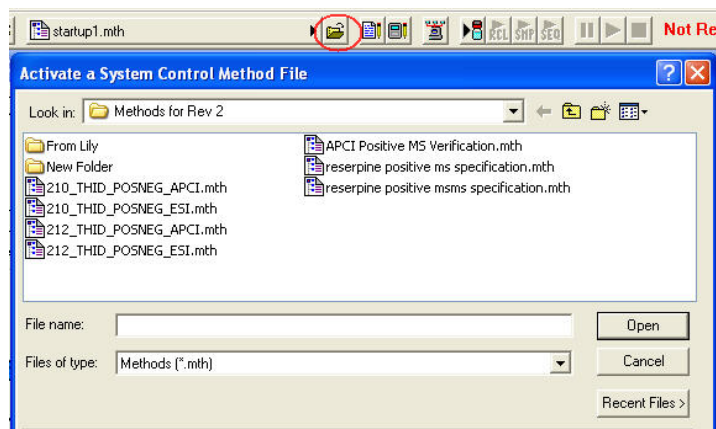
You are prompted for the name of the file to save the Method. The active Method in System Control is updated with 450-GC parameters.



The Startup Method

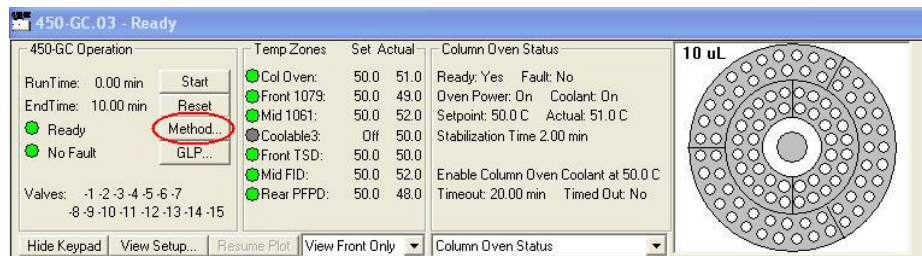
When System Control is started, the last active Method is activated and the initial settings in the Method are activated.

To change Methods, click **Activate a Method** on the System Control Toolbar.

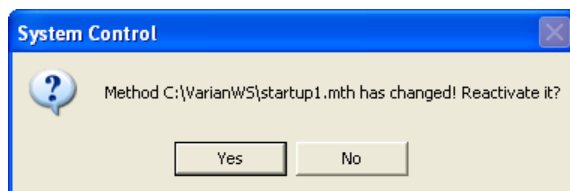


Editing 450-GC Methods

Click the **Method** button in the 450-GC Status and Control Window to open the Active Method. Any Method section can be edited.



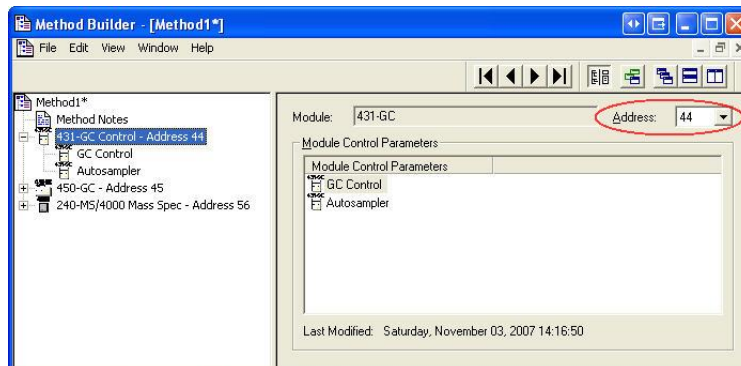
After editing the Method and closing the Method Builder window, you are prompted to reactivate the Method. Reactivating the Method downloads the changes to the Module.



431-GC Methods

431-GC Windows

Click **431-GC** in Method Builder to display the Module Control Parameters. By changing the module address in the parameter window, a method developed for an instrument using one module address can be easily modified for another instrument at a different module address.



The 431-GC Method section has two windows:

- GC Control
- Autosampler

Each window has parameters that control the GC during a chromatographic run.

431-GC Control

The GC Control window has sections for column flow, injector oven, and column oven.

Constant Column Flow Mode

Select Constant Flow **Off** to show the spreadsheet.

The first row of the spreadsheet contains the initial pressure and hold time. The instrument equilibrates to this setting when the method is activated, and is restored to this setting after each chromatographic run is completed.

The following rows contain the programmed settings for each ramp segment. Each segment ramps to the specified pressure at the specified rate (assuming the rate is achievable), and then holds the pressure for the specified time.

NOTE: The Rate field in the first row is always blank and cannot be edited. Also, the Total field cannot be edited.

Constant Column Flow Mode

Constant Flow: ☒ Off ☐ On

Column Flow (ml/min):

Pressure Pulse: ☒ No ☐ Yes

Pulse Pressure (psi):

Pulse Duration (min):

	Pressure (psi)	Rate (psi/min)	Hold (min)	Total (min)
1	10.0		20.00	20.00
2				
3				
4				
5				
6				
7				
8				

Add Insert Delete

Injector Oven

Turn the injector oven on or off, set the injector temperature, split state, and split ratio.

Column Oven Stabilization Time

The first row of the spreadsheet contains the initial temperature and hold time. The instrument equilibrates to this setting when the method is activated, and is restored to this setting after each chromatographic run is completed.

The following rows contain the programmed settings for each ramp segment. Each segment ramps to the specified temperature at the specified rate (assuming the rate is achievable), and then holds the temperature for the specified time.

NOTE: The Rate field in the first row is always blank and cannot be edited. Also, the Total field cannot be edited.

Column Oven Stabilization Time (min):

	Temp (C)	Rate (C/min)	Hold (min)	Total (min)
1	50		20.00	20.00
2				
3				
4				
5				
6				
7				
8				

Add Insert Delete

GC Autosampler

The GC autosampler window has four sections, which are similar for the 8400 and the 8410 AutoSamplers.

The parameters include the sampling syringe size, the penetration depth for sample and solvent wash vials, the default clean and clean modes, and the injection modes.

Default clean steps are used if automation is stopped or a serious fault is detected. Select Pre-Inj and Post-Inj injection syringe clean modes.

Autosampler: 8400		Sample Depth (%): 90	
Syringe Size (uL): 10 uL		Solvent Depth (%): 90	
Injection Mode: Std On Column			
Default Clean		Clean Mode	
Vial: 1	Pre-Inj Solvent Flushes: 3		
Volume (uL): 5.0	Pre-Inj Sample Flushes: 0		
Strokes: 1	Post-Inj Solvent Flushes: 1		
Speed (uL/sec): 5.0	Clean Solvent Source: 1		

Injection Mode

There are seven injection modes: Standard On-Column, Standard Split/Splitless, Neat, Viscous, and Volatile. See online Help for a detailed description of all Injection Mode parameters.

Injection Mode:	Std On Column
	Std On Column Std Split/Splitless Neat Viscous Volatile

Editing 431-GC Methods

Click the Method button in the 431-GC Status and Control Window to open the active Method and edit Method sections.

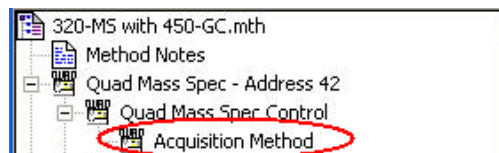
0431.02 - Ready			
0431 Operation RunTime: 0.00 min EndTime: 3.46 min Ready No Fault Start Reset Method... Setup... Extend End Stabilization Oven Off	Temp Zones Col Oven: 50 51 Heatable1: Off 50 Oven Status Column: Ready: no Fault Injector: Ready: no Fault Stabilization Time 2.00 min	Injector EFC Status Flow Ready: Yes Pressure Ready: Yes Type 1 Pressure Setpoint: 1.0 psi Actual Pressure: 0.5 psi Column Flow: 2.0 ml/min Linear Velocity: 10.0 cm/sec Total Flow: 3.0 ml/min Split State: On Split Ratio: 50	
8400: Ready	Current Vial: 1	Plunger Strokes: 510	

After editing the Method and closing the Method Builder window, you are prompted to reactivate the Method. Reactivating the Method downloads the changes to the Module.

System Control	
? Method C:\Varian\WS\startup1.mth has changed! Reactivate it?	
Yes	No

Acquisition Method

Click **Acquisition Method** in the Method Builder tree.



You can set scan segments and define MS experiments. The Mass List has a toolbar that makes completing the table like using a spreadsheet.

Method Specs.

Model: 320(GC&LC)

Ionization: ESI

Method run time: ☐ Use run time

Data type: ☒ Centroid ☐ Profile

Collect delay: ☒ Use delay 0.0 Min.

☒ Display collected file in Chro

Detector: ☐ Use EDR ☐ EDR Maximum ☒ 1000.0 Volt

☒ Detector off at method end

Scan width in SIM and MRM mode: 0.70 amu

No overrides in effect

Advanced Options

Schedule MRMs

Time segment 1 of 1

Start at retention time: 0.00 Min. Scan Channel Validation: Enabled

☒ Collect Data ☐ CID gas on

Scan Time (in Seconds): 0.500

Mass peak width in amu:

Quad 1: Calibrated Quad 3: Calibrated Copy to all

Mass List

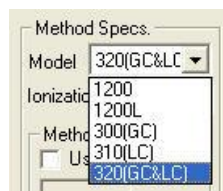
	CAS Number	Compound Name	Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Req. Dwell Time
1			Pos.	10.00	20.00					0.500
2			Pos.							
3			Pos.							
4			Pos.							
5			Pos.							
6			Pos.							
7			Pos.							
8			Pos.							
9			Pos.							
10			Pos.							
11			Pos.							
12			Pos.							
13			Pos.							
14			Pos.							
15			Pos.							
16			Pos.							
17			Pos.							
18			Pos.							

Method Specifications

The following describe the Method Specifications in the Acquisition Method.

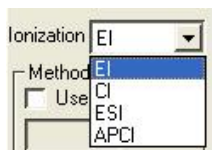
Model

Select your instrument Model.



Ionization

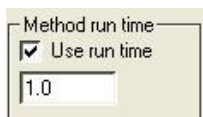
Select the ionization mode: Electron Ionization (EI), Chemical Ionization (CI), Electrospray Ionization (ESI), or Atmospheric Pressure Chemical Ionization (APCI).



Method Run Time

There are two selections:

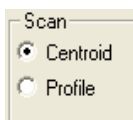
- Select **Use run time** to use the run time in the method.
- Type in the minutes to use a time other than that in the method. If you do not enter a run time, the data is acquired until the end time is reached in all other modules.



Data Type

Set the scan type (Centroid or Profile).

NOTE: Quantitation can be done in either Profile or Centroid mode.

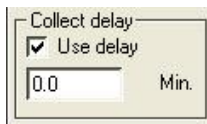


Collect Delay

This feature is useful for applications that have an initial clean up step.

To delay data collection after the run starts, do the following:

1. Check **Use delay**.
2. Enter a time in minutes. The delay time begins when the run starts.



Display File in Chro

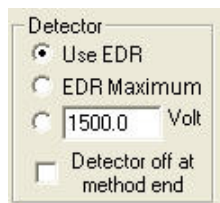
Enable to display data files in the Chro view.



Detector

- **Use EDR:** (Extended dynamic range) the detector automatically adjusts the detector voltage over the dynamic range. EDR is calibrated during AutoTune (see "AutoTune Options" on page 34.)

- **EDR Maximum:** Use the optimum fixed voltage for maximum gain from the last EDR calibration (useful for low-intensity MS/MS experiments).
- **Fixed Voltage:** Enter a fixed voltage for the entire method or different ones for each segment using Advanced Options.
- The detector can be programmed to turn off when the method ends.



Detector

☒ Use EDR

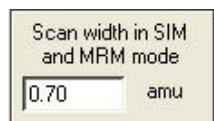
☐ EDR Maximum

☐ 1500.0 Volt

☐ Detector off at method end

Scan Width

Set the maximum peak scan window for an ion in single ion monitoring. The default value is 0.70. Increase this value to change the resolution on the scanning quad. Adjust it according to the resolution. For example, if the resolution is 3.0 on scanning quadrupole SIM width, set the SIM Width between 0.7 and 3.0 for the largest possible signal).



Scan width in SIM and MRM mode

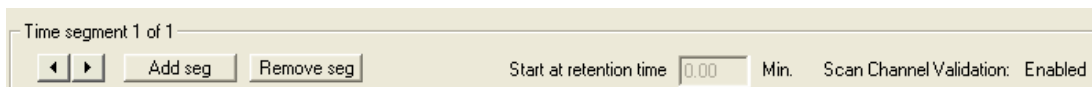
0.70 amu

Time Segment

Arrows: Use the arrows to select time segments.

Use **Add seg** to add a time segment and **Remove seg** to remove a time segment from the scan method.

Start at Retention Time defines the retention time start for each segment.



Time segment 1 of 1

◀ ▶ Add seg Remove seg

Start at retention time 0.00 Min. Scan Channel Validation: Enabled

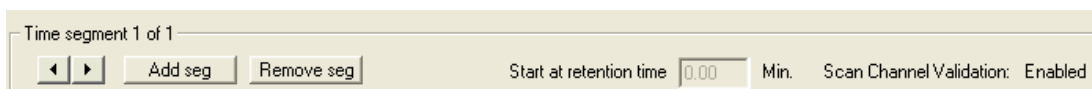
Scan Channel Validation

Validate Scan Function: Indicates if Scan Channel Validation is enabled or not. Also See MS Data Review General Preferences.

Scan Channel Validation: ensures that the scan channel specifications for all compounds are correct after transitions are added or deleted in the acquisition method.

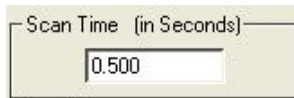
- If you change segment acquisition times, scan channel validation automatically updates the compound retention times.
- If you select a compound that specifies a deleted transition, a warning message opens. The missing transition is referred to as “255” in the compound table.
- If you process a compound table that specifies a missing transition, the following message is logged, “Invalid scan function Cannot Quantitate”.

The following shows the part of the Method Builder window that has Scan Channel Validation Enabled.



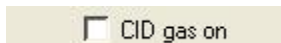
Scan Time

Set the scan speed of the MS. The scan speed is the amount of time the analyzing quadrupole does the scan. For full scan or MS/MS scan experiments, set the scan time to 0.5 seconds. More data points are acquired with shorter Scan Times. Increasing the scan time increases the signal to noise ratio since the quadrupole spends more time on the particular ion. For SIM, SRM, and MRM, decreasing the scan time allows more transitions to be scanned across a chromatographic peak.



Collision Cell Gas

Enable turn the CID gas (such as Argon) on for MS/MS operations.

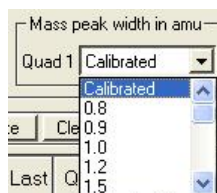


Peak Width

Set the peak width for Quadrupole 1 (Q1) or Quadrupole 3 (Q3).

Calibrated, the value from the most recent AutoTune file is the default setting and is appropriate for most applications (Scan, SIM).

For SRM and MRM reactions in MS/MS mode, the peak width of Q1 can be increased while keeping Q3 calibrated or smaller. The signal increases by allowing Q1 to transmit a wider peak width while Q3 detects the product spectra in a narrower peak.



Mass List

Enter the desired mass range (Full Scan), single masses (SIM), and precursor and product masses (MS/MS).

Q3 is used for triple quadrupole instruments only.

	Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Req. Dwell Time
1	Pos.	105.00	185.00					0.500

Ion Polarity

Click the Ion Polarity entry to switch between positive or negative ion detection. The possible ion polarity of each source is shown.

	Polarity
1	Pos.
2	Neg.

GC/MS

EI positive
CI positive and negative

LC/MS

ESI positive and negative
APCI positive and negative

Capillary

For LC/MS instruments only. Enter the absolute value of the Capillary volts for each ion in the scan method. Method Builder enters the correct sign.



Collision Energy

For triple quadrupole instruments only.

Determine the Collision Energy for each reaction and enter it in the Mass List. It defines collision energies in electron volts for specific MS/MS reactions used in the collision cell. (Refer to the *300 Series LC/MS and GC/MS (400 Series GC Hardware) Manual*, section “MS, and MS/MS”).

Collision Energy
5.000

Requested Dwell Time

Specify the Requested dwell time of each scan channel. The shorter the dwell time the greater the number of data points for the transition. Specify either the scan time or the dwell time. If there are multiple full scan ranges in a single method segment, they must all scan at the same rate; despite the requested dwell time. The software gives each mass range a dwell time according to the overall Scan Time and the relative sizes of each full scan range.

Req. Dwell Time
0.500

Mass List Toolbar

Enter values in the Mass List in a similar manner as a spreadsheet. The options are Add, Insert, Delete, or Clear All lines; Cut, Copy, or Paste from a cell or a line. Other options are fill down a column, and fill down or increment the values in a column (FD and I). The Mass List can be copied to or from an Excel spreadsheet.

Mass List									
Add	Insert	Delete	Clear All	Cut	Copy	Paste	Fill Down	FD and I	

Advanced Options

Use Advanced Options to access parameters for other features. These vary by ionization mode, instrument, and the optional ion sources (APCI and DIP/DEP probe). Use overrides when doing MS/MS breakdown curves. This provides a setpoint for the system to check.

The advanced options available depend on the ionization mode.

EI - EI Overrides, Probe, User Analogs In/Out, PMLs.

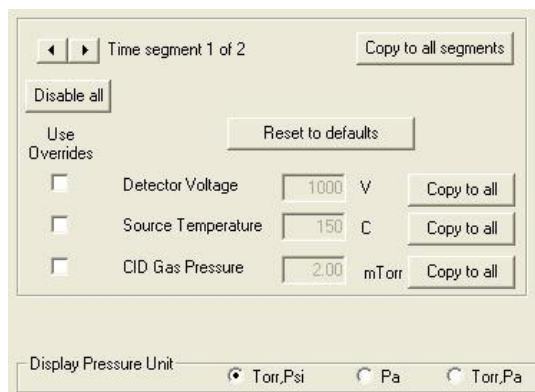
CI - CI Overrides, Probe, CI Gas Type, User Analogs In/Out, PMLs, Probe.

ESI - ESI Overrides, Valve, and Syringe Pump, Drying Gas, User Analogs In/Out, PMLs.

APCI - APCI Overrides, Valve, and Syringe Pump, Drying Gas, Vaporizer Gas, User Analogs In/Out, PMLs.

EI Overrides

Enter values to override those specified in the method for specific time segments. In the bottom section, select the units for the pressure displayed.



Time segment 1 of 2 Copy to all segments

Disable all

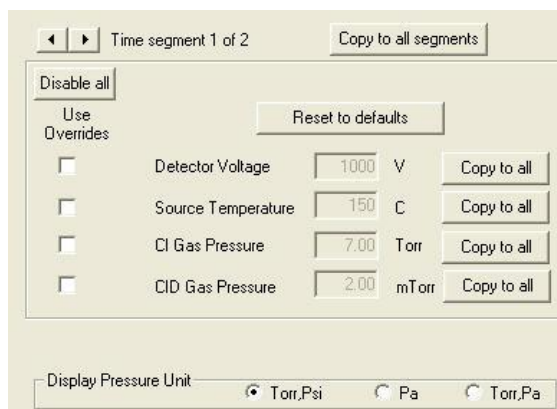
Use Overrides Reset to defaults

☐	Detector Voltage	1000	V	Copy to all
☐	Source Temperature	150	C	Copy to all
☐	CID Gas Pressure	2.00	mTorr	Copy to all

Display Pressure Unit ☒ Torr, Psi ☐ Pa ☐ Torr, Pa

CI Overrides

Enter values to override those specified in the method for specific time segments.



Time segment 1 of 2 Copy to all segments

Disable all

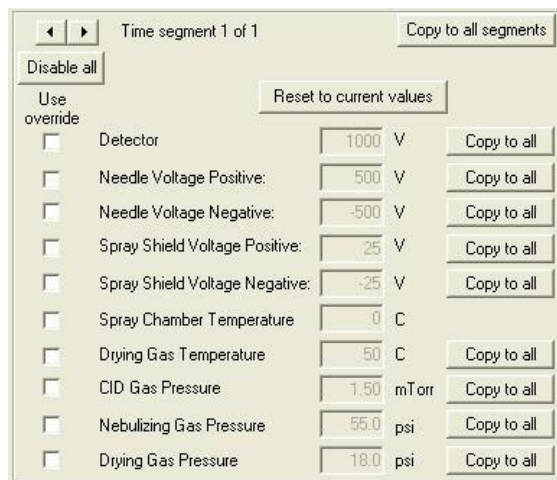
Use Overrides Reset to defaults

☐	Detector Voltage	1000	V	Copy to all
☐	Source Temperature	150	C	Copy to all
☐	CI Gas Pressure	7.00	Torr	Copy to all
☐	CID Gas Pressure	2.00	mTorr	Copy to all

Display Pressure Unit ☒ Torr, Psi ☐ Pa ☐ Torr, Pa

ESI Overrides

Enter values to override those specified in the method for specific time segments.



Time segment 1 of 1 Copy to all segments

Disable all

Use override Reset to current values

☐	Detector	1000	V	Copy to all
☐	Needle Voltage Positive:	500	V	Copy to all
☐	Needle Voltage Negative:	-500	V	Copy to all
☐	Spray Shield Voltage Positive:	25	V	Copy to all
☐	Spray Shield Voltage Negative:	-25	V	Copy to all
☐	Spray Chamber Temperature	0	C	
☐	Drying Gas Temperature	50	C	Copy to all
☐	CID Gas Pressure	1.50	mTorr	Copy to all
☐	Nebulizing Gas Pressure	55.0	psi	Copy to all
☐	Drying Gas Pressure	18.0	psi	Copy to all

APCI Overrides

Enter values to override those specified in the method for specific time segments.

Time segment 1 of 1

Copy to all segments

Disable all

Use override

Reset to current values

☐	Detector	1000	V	Copy to all
☐	Corona Current Positive:	1.00	uA	Copy to all
☐	Corona Current Negative:	-1.00	uA	Copy to all
☐	Spray Shield Voltage Positive:	25	V	Copy to all
☐	Spray Shield Voltage Negative:	-25	V	Copy to all
☐	Spray Chamber Temperature	0	C	
☐	Drying Gas Temperature	50	C	Copy to all
☐	Vaporizer Gas Temperature	50	C	Copy to all
☐	CID Gas Pressure	1.50	mTorr	Copy to all
☐	Nebulizing Gas Pressure	55.0	psi	Copy to all
☐	Drying Gas Pressure	18.0	psi	Copy to all
☐	Vaporizer Gas Pressure	18.0	psi	Copy to all

NOTE: If a multi-segment method with a temperature ramp is in progress and there is a segment with a temperature override, the temperature goes to the setpoint for that segment. The ramp continues after the segment is completed.

User Analog In/Outs

Use the Analog outputs to send the TIC signal to another device such as a LIMS system.

Use the User Input Traces to acquire data from another detector such as an Evaporative Light Scattering Detector.

Analog output #1 (User I/O connector-> Signal = pin 14 , Gnd = pin 32 +/-5 Volts)

☒ No output

☐ Output TIC

☐ Output TIC x 10

☐ Output TIC x 100

☐ Output TIC x 1000

Analog output #2 (User I/O connector-> Signal = pin 33 , Gnd = pin 15 +/-5 Volts)

☒ No output

☐ Output TIC x 1

☐ Output TIC x 10

☐ Output TIC x 100

☐ Output TIC x 1000

Collect User Traces

☐ User Input 1 Chro label:

☐ User Input 2 Chro label:

☐ User Input 3 Chro label:

☐ Readback Chro label:

☐ PML Chro label:

PMLs (Paw Macro Language)

MS Workstation provides PML macros you can use before or after a time segment. Modify and create PMLs through Tools in the Quad Module View.

The screenshot shows a dialog box titled "PMLs to be executed at each Retention Time Segment". It contains two sections. The first section, "PMLs to be executed at each Retention Time Segment", has a "Time segment 1 of 1" label, a "Copy to all" button, and a text input field with a "Browse" button. The second section, "PML to be executed after the file is collected", has a text input field with a "Browse" button.

CI Gas Type

Select the Gas Type. You can also specify another gas that is configured with your instrument.

The screenshot shows a dialog box titled "CI Gas Type". It contains four radio button options: "Methane", "Isobutane", "Ammonia", and "Other". The "Other" option is selected, and there is a text input field next to it.

ESI and APCI: Valve and Syringe Pump

For the 320-MS, Use the six-port valve or the syringe pump or both. The six-port valve can be used in Manual, Diverter or Injector mode. Set the flow rate for the syringe pump.

The screenshot shows a dialog box titled "ESI and APCI: Valve and Syringe Pump". It contains two sections. The first section, "Use of the Six-Port Valve", has three radio button options: "Manual", "Diverter", and "Injector". The "Manual" option is selected. There is also a checkbox labeled "Load position required for ready state". The second section, "Syringe Pump", has a checkbox labeled "Use Syringe Pump". Below this is a "Flow Rate" label, a text input field with the value "1.00", and the unit "uL/min". There is also a checkbox labeled "Turn off at end of method".

ESI and APCI Drying Gas

Use the SelecTemp™ feature to ensure the optimum drying gas temperature for the mobile phase composition of ESI or APCI runs.

NOTE: If a multi-segment method with a temperature ramp is in progress and there is a segment with a temperature override, the temperature goes to the setpoint for that segment. The ramp continues after the segment is completed.

Drying Gas Temperature Program

☐ Drying Gas Temperature Program in use

Temperatures (°C)		Times (minutes)
Initial temp		Initial Time
200.0		0.0
Rate (°C / min)	Final temp.	Hold Time

Total run time: 0.0 Min.

APCI Vaporizer Gas Temperature Ramp

Enter a vaporizer gas temperature program to ensure the optimum vaporizer temperature for APCI runs.

Vaporizer Gas Temperature Program

☐ Vaporizer Gas Temperature Program in use

Temperatures (°C)		Times (minutes)
Initial temp		Initial Time
100.0		0.0
Rate (°C / min)	Final temp.	Hold Time

Total run time: 0.0 Min.

DIP/DEP (Optional GC/MS Ion Source)

Enter parameters for either direct insertion probe or the direct exposure probe. See the DIP/DEP manual for more information.

Probe : From Active Method

Probe Type
Hardware Method
☒ Exposure probe
☐ Insertion probe

Current range: 0 to 1500 mA
Rate range: 2 - 2000 mA/min

Constant current
☐ Constant current 50 mA

Programmed
☐ Use

	Initial curr (mA)	Hold time (min)
Seg 1	0	0.00
Seg 2		

Rate (mA/min) End curr (mA) Hold time (min)

Total time: 0.0 minutes

Standby current
☒ Enable Standby
0 mA

Quick Start

Save
Restore

Changes current ramp to reach target ion signal strength
☒ Use

Initial probe current 10 mA
Final probe current 400 mA
Maximum ramp rate 100 mA/min
Target ion signal strength 10.0 % full scale

Ion signal type
☐ Intensity of ions scanned
☒ Intensity of mass 50.0 to 300.0

Apply OK Cancel

Schedule tMRM

Use timed MRM transitions (tMRM™) transitions to automatically break up an acquisition method into multiple segments. Using many segments in an acquisition method allows for longer MRM dwell times and therefore increases the sensitivity. See the Scheduling Timed MRM Transitions section on page 72 for more information.

Setting up MS and MS/MS Acquisitions

Overview

MS Operations

- Line 1 - Single Ion Monitoring (SIM) of 250
- Line 2 - Full Scan from 100 to 300

		Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Req. Dwell Time
SIM	1	Pos.	250.00				80.000		0.500
	2	Pos.	100.00	300.00			100.000		0.100

MS/MS Operations

- Line 1 - Selected Reaction Monitoring (SRM)
- Line 2 - Precursor Scan
- Line 3 - Neutral Loss Scan
- Line 4 - Product Ion Scan

		Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Req. Dwell Time
SRM Precursor Neutral Loss Product Ion	1	Pos.	260.00		187.00		80.000	5.000	0.500
	2	Pos.	50.00	400.00	95.00		100.000	10.000	0.100
	3	Pos.	100.00	300.00	82.00	282.00	30.000	12.000	0.100
	4	Pos.	219.00		50.00	250.00	30.000	5.000	0.100

MS Operations

Full Scan Acquisition: Scan for all ions over a defined mass range. Enter the start and end masses.

Example:

- Line 1: EI Full Scan, from mass 130 to 280

	Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Req. Dwell Time
1	Pos.	130.00	280.00					1.063

Single Ion Monitoring (SIM): Detect one or several ions. This mode is more sensitive than Full Scan.

Example:

- Line 1 - Negative SIM 321
- Line 2 - Negative SIM 414

	Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Req. Dwell Time
1	Neg.	321.00						0.500
2	Neg.	414.00						0.100

Mixed Scan Operations: Acquire data in Full Scan and SIM mode at the same time.

Example:

- Line 1: Positive SIM 120
- Line 2: Positive SIM 230
- Line 3: Positive Full Scan from 200 to 400

	Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Req. Dwell Time
1	Pos.	120.00						0.130
2	Pos.	230.00						0.130
3	Pos.	200.00	400.00					0.130

Mixed Polarity Operations: Acquire data in positive and negative ion modes for ESI and APCI.

Example:

- Line 1 - Positive SIM 120
- Line 2 - Positive Scan from 200 to 400
- Line 3 - Negative SIM 230
- Line 4 - Negative SIM 290

	Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Req. Dwell Time
1	Pos.	120.00						0.130
2	Pos.	200.00	400.00					0.130
3	Neg.	230.00						0.130
4	Neg.	290.00						0.130

Multiple Time Windows: Several time windows (Segments) can be created for an acquisition. You can do any of the previous scan modes, or mixed scan modes in any time segment and select either positive or negative polarity.

Scan Channel Validation: Enable or disable in MS Data Review as follows.

1. From **MS Data Review**, click **Preferences** and then select **General**.
2. Open the **Validation** tab, and select the **Validate Scan Functions** check box or click to clear it.
 - Enabled: If you change the time for the start at retention time value, validation will shift the retention times of all peaks proportionally.
 - Disabled: Changes you make will not be in sync.

Time segment 1 of 1

◀ ▶ Add seg Remove seg Start at retention time 0.00 Min. Scan Channel Validation: Enabled

MS/MS Operations

Product Ion Scan : Scan for fragments of a particular ion. The precursor ion is selected in Q1. In Q3 the start and end masses set the scan range for the product ions.

Example: Precursor ion 219, Product scan 50 -250, and Collision energy of 5.

	Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Req. Dwell Time
1	Pos.	219.00		50.00	250.00		5.000	0.500

Precursor Ion Scan: The precursor ions of a selected product ion are scanned. A start and end mass is set in Q1 and Q3 is set to the desired product ion.

Example: Precursor scan 100-500, Product ion 195, and a Collision energy of 10.

	Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Req. Dwell Time
1	Pos.	100.00	500.00	195.00			10.000	0.500

Neutral Loss Scan: Precursor ions are scanned in Q1. Q3 scans the same range minus the neutral loss mass.

Example: For loss of m/z 18 (water); precursor scan 100-300, product scan 82-282. Scan displays product ions resulting from the precursor ions losing a neutral mass of 18.

	Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Req. Dwell Time
1	Pos.	100.00	300.00	82.00	282.00		5.000	0.500

Selected Reaction Monitoring (SRM): This process monitors one or more MS/MS transition(s) of a precursor ion fragmenting with a specific energy into a product ion. The example shows a single transition although more can be monitored.

Example: Precursor ion 414, Product ion 219, and Collision energy -10.

	Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Req. Dwell Time
1	Pos.	414.00		219.00			10.000	0.500

Multiple Reaction Monitoring (MRM): Multiple reaction monitoring is set up like selected reaction monitoring but allows many MS/MS transitions between Q1 and Q3 to be monitored. Set the Requested Dwell Time to allow for full monitoring.

Example:

Line 1: Positive SIM: Precursor 452, Product 225

Line 2: Positive SIM: Precursor 525, Product 315

Line 3: Positive SIM: Precursor 633, Product 380

	Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Req. Dwell Time
1	Pos.	452.00		225.00			5.000	0.500
2	Pos.	525.00		315.00			10.000	0.100
3	Pos.	633.00		380.00			15.000	0.100

Mixed Polarity MS/MS Operations: Acquisition of MRM in positive and negative ion mode.

Example:

Line 1: Positive SIM: Precursor 480, Product 225

Line 2: Negative SIM: Precursor 612, Product 375

Line 3: Positive SIM: Precursor 452, Product 225

Line 4: Negative SIM: Precursor 688, Product 315

	Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Req. Dwell Time
1	Pos.	480.00		225.00			5.000	0.500
2	Neg.	612.00		375.00			20.000	0.100
3	Pos.	452.00		225.00			5.000	0.100
4	Neg.	688.00		315.00			15.000	0.100

Multiple Time Windows: Several time windows can be set within one acquisition. Each time window can allow Full Scan, SIM, MS/MS, or mixed operations and the Request Dwell time can be set appropriately.

Scan Channel Validation: Enable or disable in MS Data Review as follows.

1. From MS Data Review, click Preferences and then select General.
2. Open the Validation tab, and select the Validate Scan Functions check box or click to clear it.
 - Enabled: If you change the time for the start at retention time value, validation will shift the retention times of all peaks proportionally.
 - Disabled: Changes you make will not be in sync.

Time segment 1 of 1

◀ ▶ Add seg Remove seg Start at retention time 0.00 Min. Scan Channel Validation: Enabled

Scheduling Timed MRM Transitions

Overview

Use timed MRM transitions (tMRM™) transitions to automatically break up an acquisition method into multiple segments. The use of many segments in an acquisition method allows for longer MRM dwell times and therefore increases the sensitivity.

Before you use tMRM, enable the Scan Channel Validation option in the Validation tab of the MS Data Review Preferences General dialog.

You can schedule timed MRM transitions by filling in a blank template or by exporting the MRM data from an existing method. The following describes both:

- To create timed MRM transitions from Method Builder or System Control: In **Method Builder**, select **Acquisition Method**, and then click **Schedule tMRM** to open the **Schedule tMRM** window.
- To create timed MRM transitions from the System Control Quad Module window: Click the **Define Scan method** icon. When the window opens, click the **Schedule tMRM** button in the lower left.

The Schedule tMRM window has the following four areas:

- Create a tMRM spreadsheet template:
Create a tab-delimited *.txt file to use as a template in Microsoft Excel® to enter the tMRM transitions.
- Export a Scan Method to a tMRM spreadsheet:
Export an existing method (*.mth) to a tab-delimited *.txt file
- Import MRMs to Scan Method:
Import a text file (*.txt) with MRM data from Microsoft Excel into Method Builder.
- MRM Import Statistics:
Summary information about the last tMRM import action performed.

NOTE: After a method is created with tMRM, make additional changes to the *.txt file and import it again with tMRM.

Method Specs.

Model 320(GC&LC)

Ionization ESI

Method run time
☐ Use run time

Data type
☒ Centroid
☐ Profile

Collect delay
☒ Use delay
 0.0 Min.

☒ Display collected file in Chro

Detector
☐ Use EDR
☐ EDR Maximum
☒ 1000.0 Volt
☒ Detector off at method end

Scan width in SIM and MRM mode
 0.70 amu

No overrides in effect

Advanced Options

Schedule tMRM

Schedule tMRM (TM)

Create a tMRM spreadsheet template
 Click 'Make template' to create a blank spreadsheet Make template

Export a Scan Method to a tMRM spreadsheet
 Select a Scan Method to export and click 'Export' Export
☐ Current method
☒ Method file Browse

Import MRMs to Scan Method
 Select a tMRM spreadsheet, define parameters, and click 'Import' Import
 Spreadsheet file Browse
☒ Requested scan time 2.000 Seconds
☐ Requested dwell time 0.010 Seconds
 Minimum segment time width 0.500 Minutes
 Maximum number of segments 60

MRM Import Statistics

Number of SIM or MRM's in file:	0
Number of time segments:	0
Total acquisition time:	0.00 Minutes
Maximum scan time:	0.002 Seconds
Maximum dwell time per MRM:	0.002 Seconds
Minimum dwell time per MRM:	14,000 Seconds

Help Close

Click **Help** to open a window that outlines how to create a tMRM.

Schedule tMRM (TM) Help

To use the tMRM feature, complete the following:

- 1) Create a tMRM Spreadsheet
 - a. To create a blank tMRM spreadsheet from scratch, click on the "Make Template" button.
 - b. To extract transitions from an existing method, select a Method and click on the "Export" button.
- 2) Add MRMs to the Spreadsheet
 - a. Open the tMRM Spreadsheet in Excel® and fill in the missing data for each transition.
 - b. Save the spreadsheet database as a tab-delimited text file.
- 3) Import MRMs to Scan Method from Spreadsheet
 - a. Select the input spreadsheet name in the "Import MRMs to Scan Method" File name box.
 - b. Select either Scan Time or Dwell Time and fill in the relevant fields.
 - c. Click on the "Import" button to load the MRMs into the Scan Method.

The columns that must be defined in the tMRM Spreadsheet are:
 CAS Number, Compound Name, Polarity (+/-),
 Q1 First Mass, Q1 Last Mass, Q3 First Mass, Q3 Last Mass,
 Capillary (V), Collision Energy (V), Dwell Factor (scalar),
 Retention time (min.), RT Window width (min.)

OK

NOTE: The spreadsheet must have the CAS Number, Compound Name and Last Mass columns. You do not need to enter values.

Using tMRM with a New Method

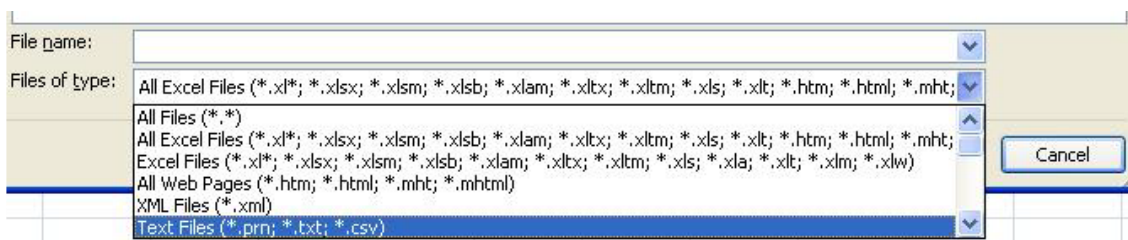
To create tMRM transitions in a blank template, complete the following two-part procedure.

1. Create and complete a new spreadsheet template, using the Create a tMRM spreadsheet template area.
2. Import the spreadsheet into a new method, using the Import MRMs to Scan Method area.

Creating a tMRM spreadsheet template

To define tMRM transitions in a new method do the following:

1. Click Make template in the Create a tMRM spreadsheet template area.
2. Enter a file name and click Save. A tab-delimited template file is saved in the VarianWS\methods folder.
3. Open Excel®, and then open the file.
4. Select Text Files in the Files of type field in the lower part of the Open window.



5. The spreadsheet has the following fields. The CAS Number, Compound Name, and the Last Mass columns are required. You do not have to put data in these three fields: the others fields must be completed.
 - CAS Number: A string containing the Chemical Abstract Services number for the compound.
 - Compound Name: A string describing the compound
 - Polarity: The polarity for acquisition method:
 - Use '+' or '-' or
 - Use the number 0 for positive and 1 for negative.
 - Q1 First Mass: The mass for Q1, m/z.
 - Q1 Last Mass: Use this only if a mass range is to be filtered in Q1, m/z.
 - Q3 First Mass: The mass for Q3, m/z.
 - Q3 Last Mass: Used only if a mass range is to be passed in Q3, m/z.
 - Capillary: Volts.
 - Collision Energy: Volts.
 - Dwell Factor: Relative factor for setting dwell times. The default is 1.
 - Requested Dwell Time: the Dwell Time is multiplied by the Dwell Factor for each transition.

- Requested Scan Time: the Dwell Time is based on the number of transitions in the segment and is multiplied by the Dwell Factor for each transition. The range is 0.006 to 14 seconds.
- Retention time: Minutes in decimal minutes. For example 1 minute and 30 seconds is 1.50 minutes.
- RT Window: Retention Time Window in decimal minutes.

	A	B	C	D	E	F	G	H	I	J	K	L
1	CAS Number	Compound Name	Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Dwell Factor	Retention time	RT Window width
2	122-39-4	Diphenylami	+	170	0	93	0	68	25.5	9.666667	0.25	0.5
3	122-39-4	Diphenylami	+	170	0	170	0	68	5	9.666667	0.25	0.5
4	60168-88-1	Fenarimol	+	331	0	189	0	105	38	9.666667	0.25	0.5

6. Complete the spreadsheet with the information for your compounds using the MRM parameters in the MRM database or another source, such as an application note, commercial or personal database. Be sure to complete the required fields.
7. Use the **Save As** command to save the spreadsheet with a new name. Keep the tab-delimited *.txt file format.

Importing MRMs to Scan Method

To import a completed MRMs spreadsheet to the scan method, do the following:

1. From the Schedule tMRM window, click Browse in the Import MRMs to Scan Method area. The Import file name window opens.
2. In the Import file name window, locate the spreadsheet, and then click Open. The file name appears in the Schedule tMRM window.
3. Select Requested scan time or Requested dwell time, and enter the time in seconds.
4. Enter the Minimum segment time width in minutes. This determines the shortest time width that tMRM uses to optimize the method. By using a smaller time width, tMRM breaks the method into more segments.
5. Enter the Maximum number of segments. This is the maximum number of segments tMRM uses to optimize the method. The maximum value is 60.

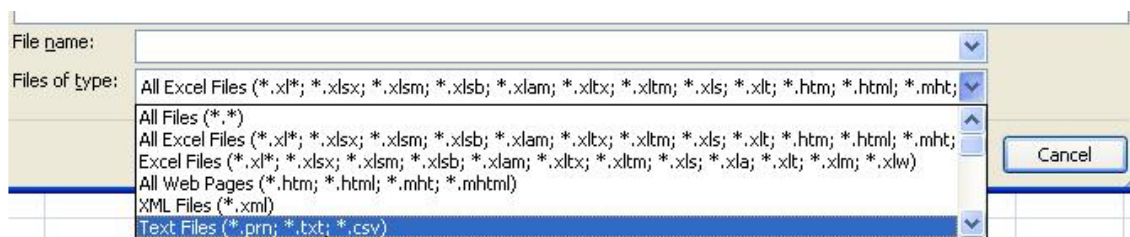
Creating tMRM transitions from an Existing Method

If you have an existing method and want to make tMRM transitions, complete the following two-part procedure.

1. To make a spreadsheet from an existing method and enter data to complete it, use the Exporting Scan Method to the MRM spreadsheet area.
2. Import the spreadsheet into a new method using the Importing MRMs to Scan Method area.

Exporting a Scan Method to a tMRM spreadsheet

1. From the Schedule tMRM window, click Browse in Export a Scan Method to a tMRM spreadsheet area.
2. Enter the file name of the existing method with the MRMs transitions, and then click Open.
3. Click Export to save the MRMs as a tab-delimited *.txt file in the VarianWS\methods directory.
4. Open Excel®, and then open the file.
5. Select Text Files in the Files of type field in the lower part of the Open window.



6. The spreadsheet has the following fields. The CAS Number, Compound Name, and the Last Mass columns are required. You do not have to put data in these three fields: the others fields must be completed.
 - CAS Number: A string containing the Chemical Abstract Services number for the compound.
 - Compound Name: A string describing the compound name.
 - Polarity: The polarity for acquisition method:
 - Use '+' or '-' or
 - Use the number 0 for positive and 1 for negative.
 - Q1 First Mass: The mass for Q1, m/z.
 - Q1 Last Mass: Use this only if a mass range is to be filtered in Q1, m/z.
 - Q3 First Mass: The mass for Q3, m/z.
 - Q3 Last Mass: Used only if a mass range is to be passed in Q3, m/z.
 - Capillary: Volts.
 - Collision Energy: Volts.
 - Dwell Factor: Relative factor for setting dwell times. The default is 1.
 - Requested Dwell Time: the Dwell Time is multiplied by the Dwell Factor for each transition.
 - Requested Scan Time: the Dwell Time is based on the number of transitions in the segment and is multiplied by the Dwell Factor for each transition. The range is 0.006 to 14 seconds.

- Retention time: Minutes in decimal minutes.
- RT Window: Retention time window in decimal minutes

	A	B	C	D	E	F	G	H	I	J	K	L
	CAS	Compound		Q1 First	Q1 Last	Q3 First	Q3 Last		Collision	Dwell	Retention	RT
1	Number	Name	Polarity	Mass	Mass	Mass	Mass	Capillary	Energy	Factor	time	Window
2	122-39-4	Diphenylami	+	170	0	93	0	68	25.5	9.666667	0.25	0.5
3	122-39-4	Diphenylami	+	170	0	170	0	68	5	9.666667	0.25	0.5
4	60168-88-1	Fenarimol	+	331	0	189	0	105	38	9.666667	0.25	0.5

- Complete the spreadsheet with the information for your compounds using the MRM parameters in the MRM database or another source, such as an application note, commercial or personal database. Be sure to complete the required fields.
- Click Save As, and then save the spreadsheet with a new name.

Importing MRMs to Scan Method

To import a completed tMRM spreadsheet to the Scan Method, do the following:

- From the Schedule tMRM window, click Browse in the Import MRMs to Scan Method area.
- In the Import file name window, locate the spreadsheet, and then click Open.
- Select either Requested scan time or Requested dwell time and enter the value in seconds.
- Enter the Minimum segment time width in minutes. This determines the shortest time width that tMRM uses to optimize the method. By using a smaller time width, tMRM breaks the method into more segments.
- Enter the Maximum number of segments. This is the maximum number of segments tMRM uses to optimize the method. The maximum acceptable value is 60.

Statistics

The Statistics area displays summary information about the most recent tMRM that was imported.

MRM Import Statistics		
Number of SIM or MRM's in file:	0	
Number of time segments:	0	
Total acquisition time:	0.00	Minutes
Maximum scan time:	0.002	Seconds
Maximum dwell time per MRM:	0.002	Seconds
Minimum dwell time per MRM:	14.000	Seconds

Injecting Samples

This section explains doing a single manual injection and programming multiple injections using the autosampler

To make a single injection, use Inject Single Sample.

To program multiple injections, use SampleList.

Overview

Samples are injected using System Control. There are four steps in data acquisition:

1. Create or modify an existing method.
2. Set up a SampleList or enter sample information for a single sample.
3. Prepare and load the samples on the autosampler.
4. Start the run.

Startup / Shutdown of LC/MS

The startup and shutdown procedures and the injection methods are the same for both the Electrospray Ionization (ESI) and Atmospheric Pressure Chemical Ionization (APCI) methods.

Startup

The instrument must be pumped down and running before you begin.

1. Click **Turn Spray On** in the Quad View to turn on the gasses and heaters.
2. After the Drying gas temperature reaches at least 75% of the set value, start the LC pumps.
3. Wait a few minutes for the temperature to stabilize and click **Analyzer On/Off** to turn on the Detector.



Shutdown

1. Turn off the LC pumps.
2. Allow the LC pump pressure to drop down and stabilize so the flow into the MS stops. Click the **Spray icon** to turn off the gasses and heaters. The Analyzer turns off automatically when you turn off the source.

320-MS LC/MS Syringe Pump and Valve

Use the six port valve to divert flow away from the 320-MS, or to make injections. Set the flow of the syringe pump and have the pump shut off at the end of the method.

See the *300 Series LC/MS and GC/MS (400 Series GC) Quadrupole Manual* to set up the syringe pump.

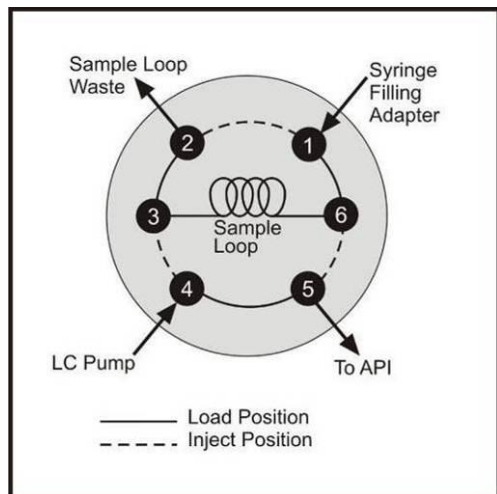
1. Click **Advanced Options** and select the **Valve and Syringe Pump** tab.
2. Select **Manual**, **Diverter**, or **Injector** for the valve. The system can turn the syringe pump off at the end of the run.
3. Enable **Use Syringe Pump**, type in the flow rate, and enable the check box **Turn off at end of method**.

The screenshot shows the 'Advanced Options' dialog box with the 'Valve and Syringe Pump' tab selected. The dialog has a blue title bar with a close button. Below the title bar is a tabbed interface with five tabs: 'Overrides', 'Valve and Syringe Pump', 'Drying Gas', 'User Analogs In/Out', and 'PMLs'. The 'Valve and Syringe Pump' tab is active. Inside this tab, there are two main sections. The first section, 'Use of the Six-Port Valve', contains three radio buttons: 'Manual' (selected), 'Diverter', and 'Injector'. Below these is a checkbox labeled 'Load position required for ready state'. The second section, 'Syringe Pump', contains a checkbox 'Use Syringe Pump' which is checked. Below this is a 'Flow Rate' field with the value '50' and the unit 'uL/min'. At the bottom of this section is a checkbox 'Turn off at end of method' which is also checked. At the very bottom of the dialog are 'OK' and 'Cancel' buttons.

LC/MS Manual Injections

Manual Injection

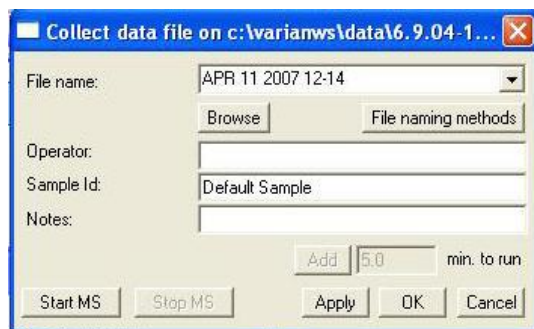
Plumb the switching valve as shown.



To do manual injections do the following:

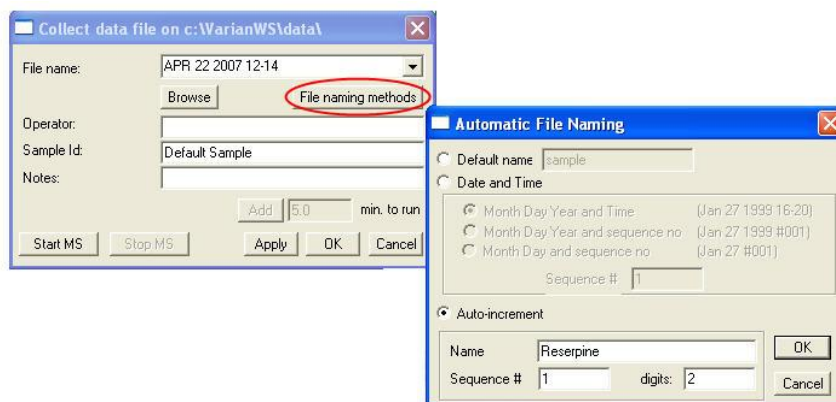
1. Monitor the baseline using the **Plot Tic** tool in the **Tools** menu.
2. After the baseline stabilizes, click the **Traffic light** and the **Collect data file** window opens.

NOTE: The source and detector must be on to use the Traffic light to collect data.

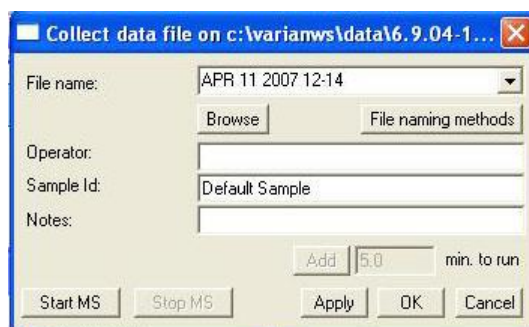


3. Click **File naming methods** to open the **Automatic File Naming** window.
4. Click **Auto-increment**. Type in the name of the data file.
5. Enter **1** for Sequence #, and **2** for digits.

NOTE: Click **Browse** to review or select an existing file name that you may wish to use as a root for the file name of your sample.



6. Click **OK** and the **Automatic File Naming** window closes.

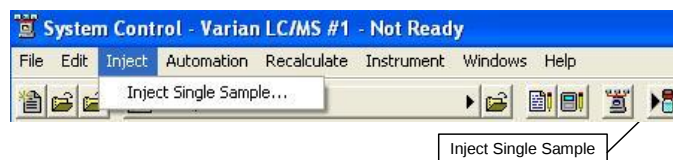


7. Complete the **Collect data** window.
8. Click **Apply** and if you are ready to collect data, click **Start MS**.
9. Check that the valve is in the load position.
10. Overfill the 5 μ L switching valve loop with 3 or 4 times the volume. Push the button on the valve cover. Allow at least 1 minute between injections or click the valve icon in the Quad view.
11. Stop data collection by opening the Collect data window and clicking **Stop MS**.

GC/MS or LC/MS Injecting Single Samples

To do one injection, do one of the following:

- Click Inject Single Sample from the Inject menu
- Click the Inject Single Sample icon on the System Control menu bar.



Clicking **Inject Single Sample** from the Inject menu opens the following window. The fields are dependent on the sampling device. For more information about these fields, see the “SampleList and RecalcList Fields” section in the *MS Data Handling User's Guide*, part number 3954038.

The 'Inject Single Sample' dialog box contains a table with the following data:

Sample Name	Sample Type	Cal. level	Inj.	Injection Notes	AutoLink	Inj. Mode	Inj. Volume	Plate	Well / Vial
Default Sample	Analysis		1	none	none	Partial Loopfill	10.0		A1

Below the table, there is a section for 'Inject the Sample using the Method:' with a text field containing 'C:\VarianWS\startup1.mth', a 'Browse...' button, and a 'Defaults...' button. There is also a checkbox for 'Clear Coefficients before Calibrating'. At the bottom, there are 'Inject' and 'Cancel' buttons, and 'Data Files...' and 'RecalcList...' buttons.

Enter the Data File Name and Path

Data File names can have up to 255 characters. They can be a combination of Sample ID, injection date, module name, and injection number.

Click **Data Files** to open the Data Files Generation window.

The 'Data File Generation' dialog box has two main sections. The left section, 'Directory for Data Files', shows a tree view of the file system with 'c:\varianws' selected. Below it is a 'New Folder...' button and a 'Drives:' dropdown menu showing 'c:'. The right section, 'Data File names', has a text field containing '%s %d'. Below this is an 'Example:' section showing 'Sample 1 8-30-2006'. At the bottom, there is a list of symbols and their corresponding variable data: %s = Sample ID, %i = Injection number, %d = Date, %m = Detector Module name, %t = Injection Time, %h = Method Name, %o = Operator Name, %n = Instrument Name. 'OK' and 'Cancel' buttons are at the bottom.

Select the drive letter and subdirectory (path) to store your files from the left side. The default directory is the data subdirectory of your VarianWS directory.

Create a filename format on the right side. You can combine a text entry with the “%” symbols to specify filenames with variable sample injection information. An example of the filename updates as you enter filename specification.

The files the SampleList creates can be stored in a RecalcList, which tracks the names of the created files and other parameters. You can reprocess the RecalcList later, for example, to reprint the reports or to process data with another method.

RecalcList Generation

You can automatically create or update a RecalcList with files generated during automated injections. Specify the RecalcList generation options for this SampleList below.

☒ Do not automatically create and update a RecalcList.

☐ Create and update a new RecalcList.
RecalcList name:

☐ Append to an existing RecalcList.
RecalcList name:

☐ Overwrite the Recalc List each time the SampleList Begins.

Click **Append to an existing RelcalcList**, to append a number to the new RelcalcList filename.

QuickStart injects a single sample without using System Control directly.

QuickStart starts System Control and waits for all modules to log in before opening.

Enter information in the MS QuickStart window about your injection. For more information about the fields, see the “SampleList and RelcalcList Fields” section in the *MS Data Handling User’s Guide*, part number 954038.

The MS QuickStart - 1 window is a configuration interface for an autosampler. It features a menu bar with 'File', 'Screen', and 'Options'. The main area contains several input fields and controls:

- Instrument Number:** A text box containing '1'.
- Instrument Name:** A text box containing 'Instrument #1'.
- Operator Name:** A text box containing 'Operator'.
- Sample Name:** A text box containing 'Default Sample'.
- Sample Description 1:** An empty text box.
- Sample Description 2:** An empty text box.
- Primary Method:** A text box containing 'C:\VarianWS\startup1.mth'.
- Folder for Data File Storage:** A text box containing 'C:\VarianWS'.
- Browse:** A button next to the folder path.
- Sample Type:** A group box containing four radio buttons: 'Baseline', 'Calibration', 'Analysis' (selected), and 'Verification'.
- Well/Vial:** A text box containing 'A1'.
- # Injects:** A text box containing '1'.
- Wash Vol.:** A text box containing '0'.
- Volume:** A text box containing '1'.
- Amount:** A text box containing '1'.
- Factor:** A text box containing '1'.
- Multiplier:** A text box containing '1'.
- Divisor:** A text box containing '1'.
- Level:** A text box containing '1'.
- Inj. Mode:** A dropdown menu set to 'Full Loop'.
- Hardware:** A button.
- Clear Coefficients:** A checkbox that is unchecked.
- AutoLink...:** A button.
- Start:** A green button.
- Stop:** A red button.
- Help:** A button.
- Exit:** A button.

Autosampler Display

Each of the supported autosamplers has a graphic representation of the carousel or tray. In System Control, click the autosampler icon in the Instrument Status Window to open it. Inject from a vial by double-clicking on the appropriate vial in the display.

After the Inject Single Sample dialog opens, enter the information, and make the injection.

The Autosampler Display window provides a visual representation of the autosampler's state and controls for a single injection. It includes:

- Top Bar:** Displays '430.33 - Ready'.
- Left Panel:** Shows system information: 'BVP : Varian LC/MS #1', 'Free disk: 136582.09 MBytes', and a diagram of the vial tray with vials 212, 430 (highlighted), and 42. Below this, it shows 'Method: startup1.mth' and '0 injections, 0 calculations', '0 recalculations, 0 reports generated'.
- Right Panel:** Contains controls for the injection process:
 - AutoSampler Operation:** Includes 'RunTime: 0.00 min', 'EndTime: 0.00 min', 'Well: C2', 'AUX: -1 -2 -3 -4', 'P3 OUT: 0 (hex)', and status indicators for 'Ready' (green dot) and 'No Fault' (green dot).
 - Active Sample Status:** Includes fields for 'Name:', 'Location:', 'Injection:', and 'Activity:'.
 - Buttons:** 'Start', 'Reset', 'Wash', 'Method...', 'Lift', 'Plate', 'Temp: °C', 'Hide Keypad', 'Cooling On', 'Change Plate', 'Hardware...', and 'Fill Syringe'.
- Vial Tray:** A 6x6 grid of circles representing vials. Vial 430 is highlighted. A callout box points to it with the text 'Click vial'.

Running Priority Samples Using Inject Single Sample

Use either the graphical vial selection or Inject Single Sample to make a priority injection during automated analyses.

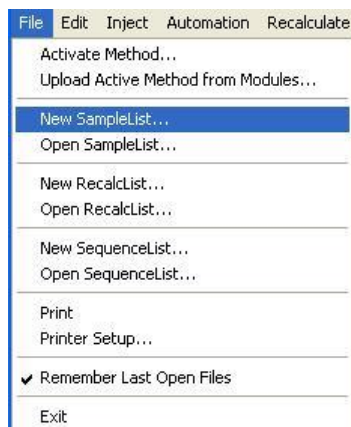
1. While automation is running, click **Suspend** on the current active SampleList. Automation is suspended after the current run is completed.
2. Double-click the **vial position** of the priority sample or choose **inject single sample**.
3. After completing the priority run, click **Resume** to re-start the SampleList.

LC/MS or GC/MS Injecting Multiple Samples

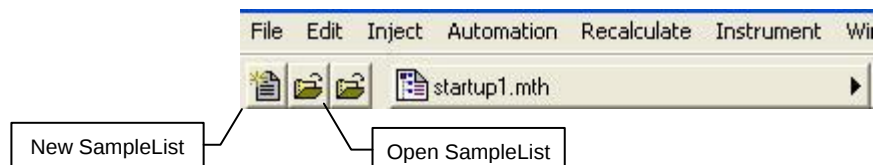
You can create SampleLists for different autosamplers, and use more than one method for your injections.

SampleLists in System Control

- To inject multiple samples from System Control, use a SampleList from the File menu or from System Control.
- To create a new SampleList: On the File menu, click **New SampleList** or click **Open SampleList** to select an existing one.
- For more information about the fields, see the “SampleList and ReclacList Fields” section in the *MS Data Handling User's Guide*, part number 954038.



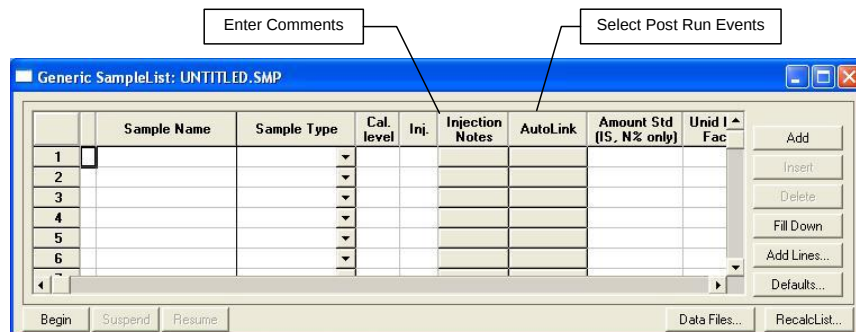
From the System Control toolbar, create a new SampleList or open an existing one



Generic SampleList

If no sampling device is configured, a generic SampleList opens. This SampleList does not have fields for vial positions, sampling options or hardware configuration options.

The SampleList fields are like spreadsheet columns and can be sized by dragging the border. Right-click a column header to display formatting options.



The Sample Name field remains fixed as you scroll to the right to help you enter information about your samples.

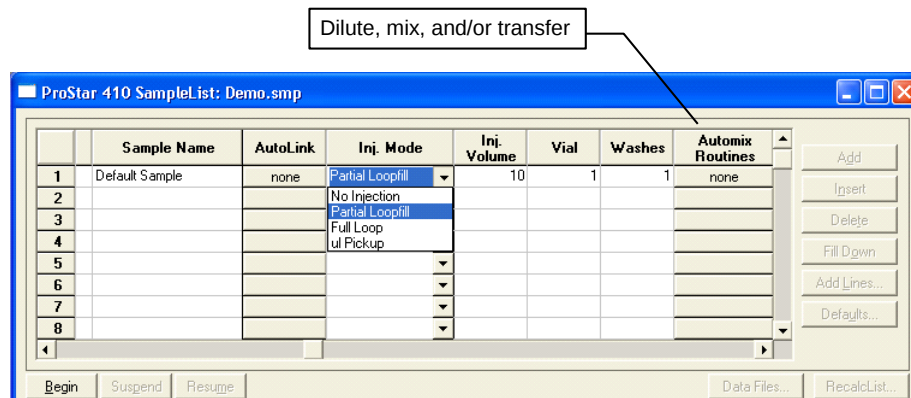
You can enter data handling parameters, such as, the amount for single internal standard calculations, the unidentified peak factor, a multiplier, and a divisor.

If your requirements are more complex (such as multiple internal standards or multiple detectors, which require different entries) use the MultiChannel MultiStandard field.

Each autosampler has a unique SampleList. A SampleList can have more than one autosampler section so it can be used with different autosamplers.

LC/MS: ProStar 410 SampleList

In addition to the Generic SampleList features, the ProStar 410 supports other features such as different Injection Modes, Vial Specification, and AutoMix functions.



Automix Steps

	Action	Amount	From	To
1	Add	10 ul	Reagent A	Sample
2	Mix	10 ul	1 time	
3	Wait	0.50 min		
4				
5				
6				
7				
8				
9				
10				

Destination Vial: none

☒ Automix First Injection Only

Ok Cancel Mix Remove Save As Default Automix Step

Add Insert Delete Import...

Click **Add Lines** to add several lines to the SampleList.

Add Lines to ProStar 410 SampleList

Sample Name	Sample Type	Cal. level	Inj.	Injection Notes	AutoLink	Inj. Mode	Inj. Volume	Vial	Washes	Automix Routines	Prep Steps	Amount Std (IS, N% only)	Unit f
Default Sample	Analysis		1	none	none	Partial Loopfill	10	1	1	none		1	0

Number of Lines to Add: 10

☒ Number Sample Names from: 1 ☒ Number Vials from: 1

Add Insert Cancel

Sequentially number Sample Names

From the ProStar 410 SampleList, Press **Begin**, and you are prompted to select a Method. Use the active Method that was, or click **Browse** to use another.

Click **OK**, to begin the run.

Begin Sample List

System Control will inject the Samples using the Method:

C:\Varian\WS\methods\420_Dynamax.mth Browse...

Data Files will be saved in:

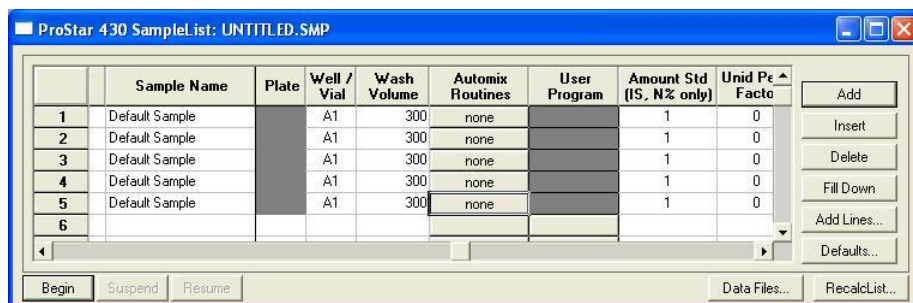
c:\varian\ws\data

OK Cancel

LC/MS: ProStar 420 and 430 SampleList

The ProStar 420 and ProStar 430 SampleLists have generic System Control SampleList fields and fields for operations specific for each AutoSampler.

To build a ProStar 420 SampleList or a ProStar 430 SampleList, click **Add**.



	Sample Name	Plate	Well / Vial	Wash Volume	Automix Routines	User Program	Amount Std (IS, N% only)	Unid Pe Facto
1	Default Sample		A1	300	none		1	0
2	Default Sample		A1	300	none		1	0
3	Default Sample		A1	300	none		1	0
4	Default Sample		A1	300	none		1	0
5	Default Sample		A1	300	none		1	0
6								

You can enter information common for all samples. You can select the number of entries to be added sequentially to the SampleList. With the ProStar 420, you can specify the first and last vials to be added to the SampleList with the requirement that the first and last vial numbers start with the same Tray Type letter, A, B, C, or D.

With the ProStar 430, you can specify the first and last Row and Column to be added. You can also select to add by Rows or Columns, which determines if the plate is processed from left to right by row or from top to bottom by columns.

Select Partial Loop fill, Full Loop, or μ L Pickup from the Injection Mode field. Select the User Program from this field also. Several fields are disabled when User Program is selected.

For the ProStar 430, use the Plate column to specify the plate that has the well or vial with the sample. Enter a plate number between 1 and 7. This field is disabled unless the ProStar 430 is equipped with the Plate Feeder option.

The ProStar 430 Well/Vial field specifies the sample location as a combination of row letter and column number. The available rows and column numbers depend on the type of plate configured.

- 48 standard vials: A1 through F8
- 96 well plate: A1 through H12
- 384 well plate: A1 through P24

Use the Well/Vial field to randomly access any well or vial. For example, you can periodically recalibrate from a single standard in a fixed location.

For the ProStar 420, the Vial field specifies the sample vial as a combination of Tray type letter and Vial number. The available Tray types and Vial numbers depend on the Tray Segments configured. You can randomly access any vial.

In the Wash Volume field enter a wash volume in the range of 300 to 9999 μ L, or enter 0 for no wash.

In the Automix Routines field, define a specific automixing program to be done before the sample is injected. When doing an Automix routine, you can program the AutoSampler to aspirate liquid from a well, vial, or a reagent vial, and transfer it to the sample well or vial from which an injection is to be made.

You can mix the sample by aspirating and dispensing specified amounts.

You can program the AutoSampler to wait for a specific time interval. Use the Automix Steps dialog to select Action, Position, Amount, Speed of the syringe, and Height of the needle. The following is an example of an Automix routine.

Automix Steps

	Action	Position	Amount	Speed	Height	Comment
1	Aspirate From	Sample	10.0 ul	3 (normal)	5 mm	
2	Dispense To	Sample	10.0 ul	3 (normal)	5 mm	
3	Aspirate From	Sample	20.0 ul	3 (normal)	5 mm	
4	Dispense To	Sample	20.0 ul	3 (normal)	5 mm	
5	Repeat		2 times		2 steps	
6	Wait		1.00 min			
7	Rinse+Wash		100.0 ul			
8						
9						
10						

Destination Well: none Destination Plate: Sample Plate

Reagent A Vial: None Reagent C Vial: None
 Reagent B Vial: None Reagent D Vial: None

☒ Automix First Injection Only Save As Default Automix Step

Ok Cancel Remove From SampleList Remove From Sample

Add
Insert
Delete
Import...

A maximum of 240 steps can be programmed in one Automix routine. After entering all the steps, enter a name for this Automix Program in the box next to Cancel and click **OK**. The program is saved in the SampleList, and can be exported to other SampleLists. Alternatively, Automix Programs from other SampleLists can be imported to the active SampleList using Import.

The User Program column is enabled if selected in the Injection Mode field for the sample. The User Program can do sample handling and injection actions.

When the User Program is selected as the Injection Mode, the following fields are disabled; Injection Volume, Wash Volume and Automix Routines. The User Program steps are used instead of the method parameters. You must use the User Program if the 10mL syringe is selected. The following figure shows lists the User Program Actions. For each specified action, there could be several options such as Position, Amounts, Speed Setting, and Height. Start the run, by selecting **Start run on the INJECT Marker** or selecting **Start run at End of User Program**.

User Program Steps

	Action	Position	Amount	Speed / Setting	Height	Comment
1	Aspirate From	Reagent A	10 ul	3 (normal)	5 mm	
2	Dispense To	Sample	10 ul	3 (normal)	5 mm	
3	Wait		1.00 min			
4	Repeat		1 times		3 steps	
5	Wash		100 ul			
6	Valve	Injector		Inject		
7	Syringe	Load	100 ul	3 (normal)		
8	Compressor			Off		
9	Set Output	INJECT				
10						

Destination Vial: none

Reagent A Vial: C30 Reagent C Vial: none
 Reagent B Vial: none Reagent D Vial: none

☒ Start Run on INJECT Marker
☐ Start Run at End of User Program Save As Default Program Step

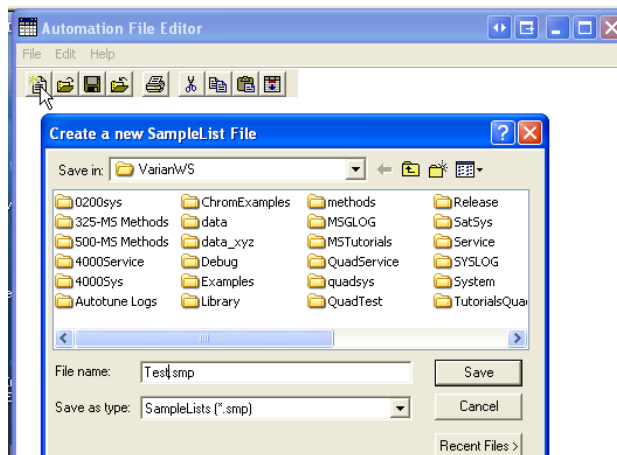
Ok Cancel UserProg_1 Remove From SampleList Remove From Sample

Add
Insert
Delete
Import...

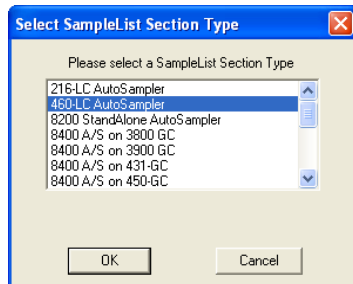
LC/MS: 460-LC SampleList

To create a 460-LC SampleList, do the following:

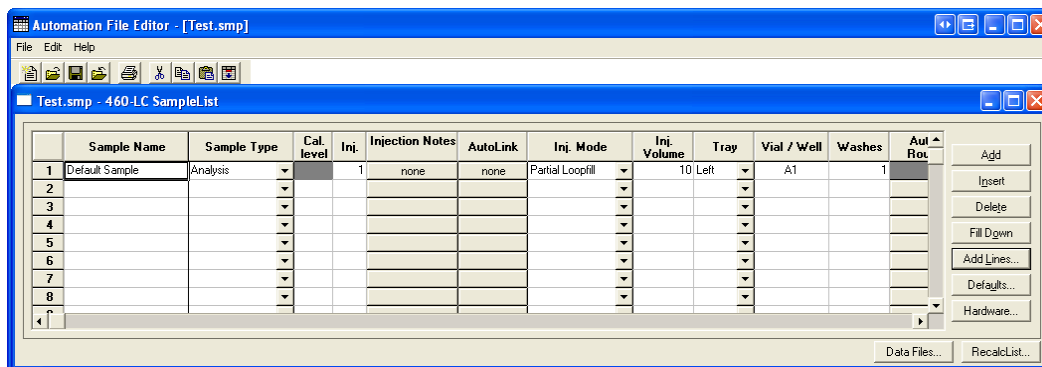
1. Click **Edit Automation Files** to open the **Automation File Editor**.
2. Click **New Automation File** and click **new SampleList**.
3. Enter a file name and click **Save**.



4. Select the **460-LC AutoSampler** and click **OK**.



5. An empty SampleList with your file name opens
 - Click **Add** to add one sample.



- Click **Add Lines** to add several samples or a plate.

- Click **Hardware** to specify the tray type for each position, sample loop volume and indicate if the Syringe for Prep Mode is installed.

Sample Name: Enter the “root” name for all samples.

Sample Type: Select **Analysis**, **Calibration**, **Verification**, or **Baseline** from the menu.

Cal. Level: This numerical field is used with Calibration and Verification Sample Types.

Inj. Enter the number of injections in this numerical field.

Injection Notes: Enter a note about the sample or the injections in this text field.

Injection Notes	
1	Test method A

AutoLink: Add a Command or Other parameters for post run event.

Injection Notes	AutoLink	Inj. Mode	Inj. Volume	Tray	Vial
Test method A	none	Partial Loopfill	10	Right	

AutoLink Parameters

Command

Other parameters

Browse...

OK

Cancel

Injection Mode: Select **No Injection**, **Partial Loopfill**, **Full Loop**, or **μL Pickup** from the menu.

Inj. Volume: The 460-LC comes with a 100 μL sample loop. Injections can be made with 1 μL increments.

Tray: Create a sample list for either the **Left** or **Right** tray.

Vial/Well: Enter a combination of a row letter and a column number. The available rows and column numbers depend on the type of plate configured.

- 96 well plate: A1 through H12
- 384 well plate: A1 through P24

Wash Volume: Enter 1 to 9 washes.

Automix Routines: Use these routines only with the 84+3 Adapter Tray.

GC/MS: CP-8400/8410 SampleList

In addition to the Generic SampleList features, the CP-8400/8410 has settings for Vial position, Injection Volume and Injector Selection. If SPME hardware is installed, the Injection Volume field is disabled and the fiber Adsorption Time set in the GC control section of the Method is used for sample extraction.

	Sample Name	AutoLink	Vial	Injection Volume	Injectors Used	Amount Std (IS, N% only)
1	Default Sample	none	0	1.0	Pos 1	1
2					Pos 1	
3					Pos 2	
4					1 then 2	
5					2 then 1	
6					Manual	

Begin

Suspend

Resume

Data Files...

RecalcList...

Select Manual from the Injectors Used field to disable the CP-8400/8410 and make a manual injection. In the following example, the CP-8400/8410 injects samples 1 and 2, then waits for a manual injection/start from the GC for sample 3, and continues with samples 4 and 5 using the CP-8400/8410.

8400 SampleList: 8400_Demo.smp

	Sample Name	AutoLink	Vial	Injection Volume	Injectors Used	Amount Std (IS, N% only)
1	sample 1	none	0	1.0	Pos 2	1
2	sample 2	none	0	1.0	Pos 2	1
3	sample 3	none	0	1.0	Manual	1
4	sample 4	none	0	1.0	Pos 2	1
5	sample 5	none	0	1.0	Pos 2	1
6						

Buttons: Add, Insert, Delete, Fill Down, Add Lines..., Defaults...

Buttons: Begin, Suspend, Resume, Data Files..., RecalcList...

The CP-8400/8410 can make two injections in the same GC method run. Select second injector from the Injectors Used field.

Injectors Used	2nd Injection	Injection Delay
1 then 2	Duplicate	0.5
	Duplicate	
	Advance	
	Clean & Dup	
	Clean & Adv	

If two injectors are used, you can do the following with the second injector, inject the same sample as the first injection (Duplicate), or inject the sample from the next vial position (Advance). You can wash the syringe in between injections (Clean & Dup, or Clean & Adv).

In the following example 1.0 μ L of Sample 1 from vial 5 is injected by injector 1, there is a 2.0 seconds delay, and 2.0 μ L of Sample 2 from vial 6 is injected by injector 2. A separate data file is created for each sample.

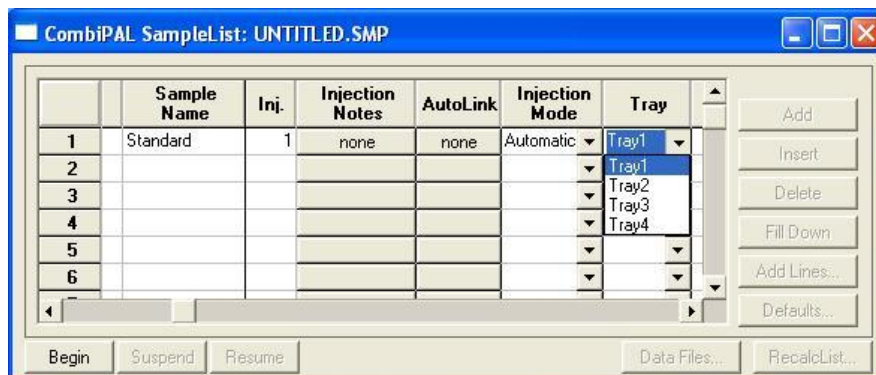
8400 SampleList: 8400_Demo.smp

	Sample Name	2nd Sample Name	AutoLink	Vial	Injection Volume	2nd Inj Volume	Injectors Used	2nd Injection	Injection Delay	A
1	Sample 1	Sample 2	none	5+6	1.0	2.0	1 then 2	Advance	2.0	
2										

Combi PAL SampleList

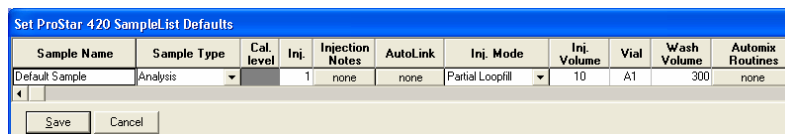
In addition to the Generic SampleList features, the Combi PAL for GC/MS and HTS PAL for LC/MS have settings for Tray selection, Vial position, and Injection Volume. If the Combi PAL is configured for SPME sampling, then the Injection Volume field is disabled and the fiber Extraction Time set in the Combi PAL control section of the Method is used for sample extraction.

All other sampling parameters are specified in the Combi PAL section of the Method.



Default SampleList Entries

When you add a new row to a SampleList, default values are entered. To change them, click **Defaults** and the **Set ProStar 420 SampleList Defaults** dialog box opens. Enter the desired default values and click **Save**.



Note that volume, rack, and vial number are not displayed, even if an AutoSampler is present.

Saving SampleLists for Later Use

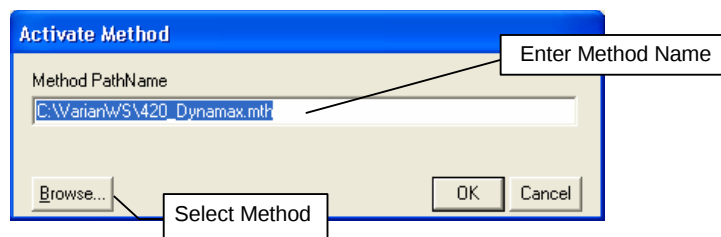
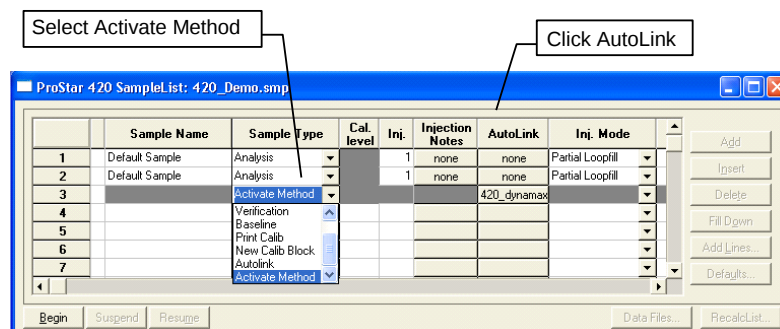
When you make changes to the open SampleList, the changes are automatically saved to the SampleList file and are used for the automated runs in progress. If you want to edit a SampleList other than the open SampleList, use the offline Automation File Editor application described in the next section of this manual.

Using More Than One Method for Injections

You can do automated injections using more than one Method. There are two ways to do this: change the active Method in the SampleList or use a SequenceList.

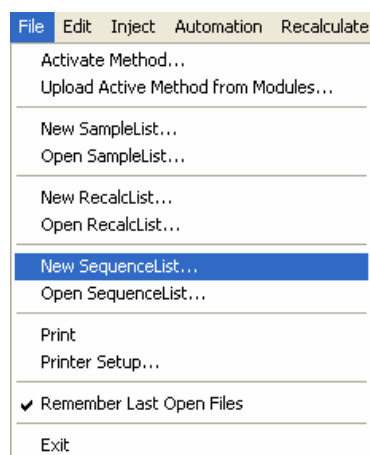
Changing the Method in the SampleList

Change the Method by activating a Method in a SampleList row.

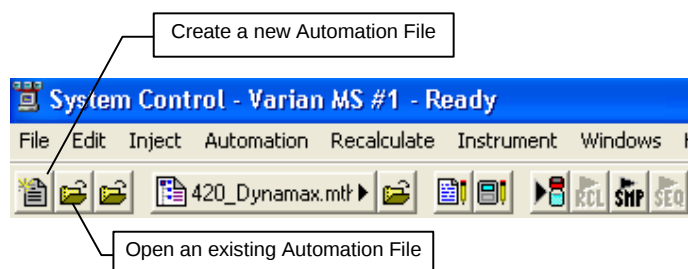


Using the SequenceList Window

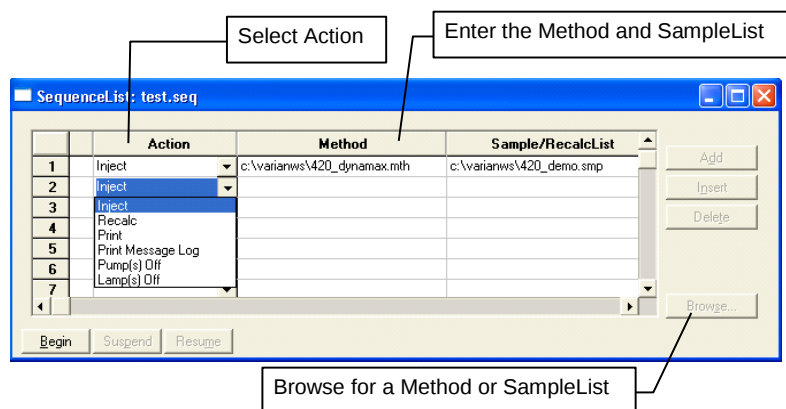
On the **File** menu, select a **New SequenceList** or **Open SequenceList**.



Create a new SequenceList or open one from the System Control toolbar.

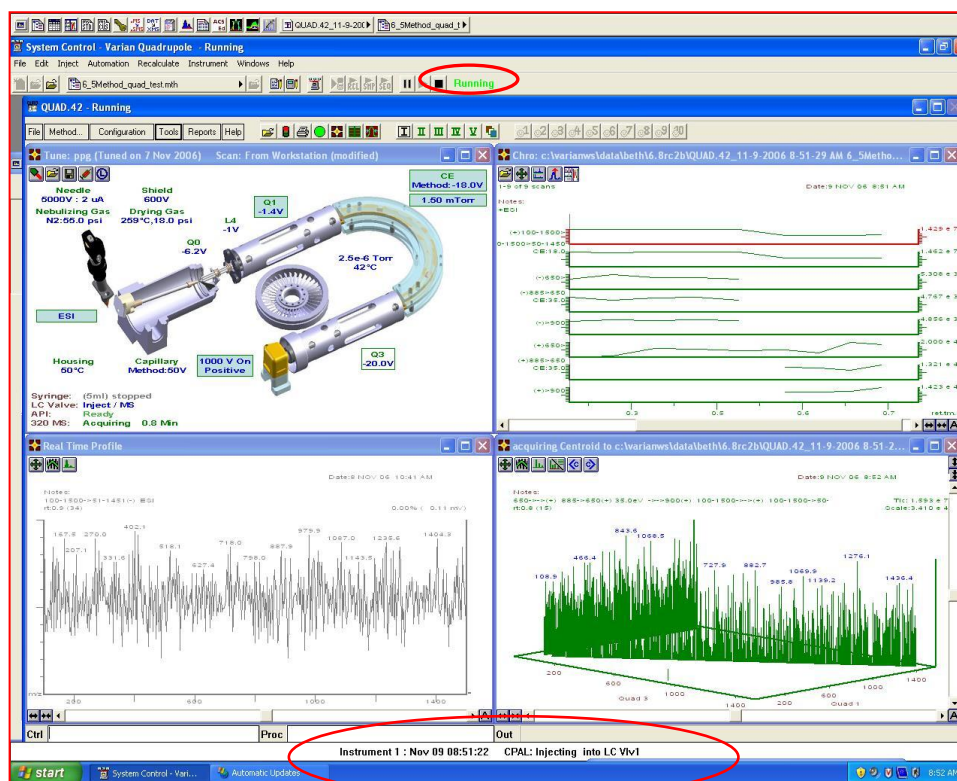


In the SequenceList, select an **Action**. Enter the **Method** and the **SampleList** or click **Browse** to select from a list.



Monitor Run Status

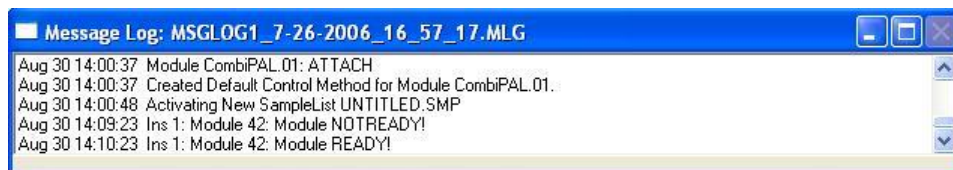
After making an injection, monitor the run in System Control.



The status and control window and the Toolbar display the module status.

Message Log

Automation actions and errors are recorded in the Message Log. The most recent entry is at the bottom. Double-click the status bar at the bottom of the instrument window to display the entire Message Log. The log is saved in the c:\VarianWS\MSGLOG directory. Each Message Log entry is stamped with the time and date.



Automated MS Report Generation

Add Report sections to your Methods to generate automated reports from System Control after each injection, after Recalculations, or by using Print actions in the Sequence window. When Automated Printing is enabled, a checkmark appears in the front of the Enable Automated Printing menu listing. To disable automated Report printing during an automated sequence of injections or Recalculations, click **Enable Automated Printing** from the Automation menu to disable it and remove the check mark. A SCII file is generated, if selected in the Report Method section. When you disable automated printing, automation continues but no reports are printed.



Stopping an Acquisition

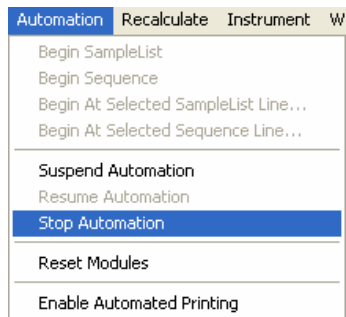
During automation and while the LC/MS or the GC/MS system is running you can suspend or stop data acquisition from the Automation menu in System Control.

Suspend Automation: Suspend automation after the current run is completed.

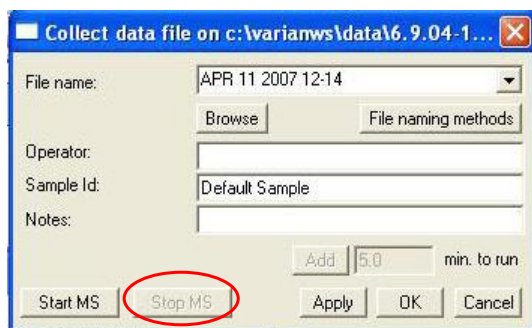
Stop Automation: Stop the current run, reset the modules, and suspends automation.

Resume Automation: Resume automation after suspension.

Reset Modules: Stop the current run, and reset all modules. Automation proceeds to the next injection after all the modules go to the Ready state.



If the Acquisition was started from Start collecting data  in the window Toolbar, click **Stop MS** to end data acquisition or in the Automation Menu bar click **Stop Automation**.



Set a Collect Delay

Use collect delay to start data acquisition after the sample is injected. A separation can be set up to remove buffer from the sample. The solvent or buffer can be diverted to waste and data collection can be started after the valve switches to bring the flow into the MS. In the first 30 seconds of a separation, data collection can be turned off while un-retained compounds that are not of interest are washed off the column. Data collection can start when the mobile phase composition changes and the sample begins to elute.

LC/MS

Divert the LC effluent away from the API Source using the 320-MS 6 port valve. Frequently, the solvent front contains un-retained non-volatile salts from the sample. If not diverted, these salts would deposit on the source and the source may require more frequent cleaning. The delay parameter switches the diverter valve to waste for a set time.

While the flow is diverted from the source, you can delay data collection in the Acquisition Method. The syringe pump can be programmed to provide make up flow to the API while the LC effluent is diverted.

GC/MS

Use the Delay parameter to turn the filaments on after a time interval. Use this in GC/MS runs to prevent the filaments from being damaged or broken while the solvent peak elutes.

Acquisition Method

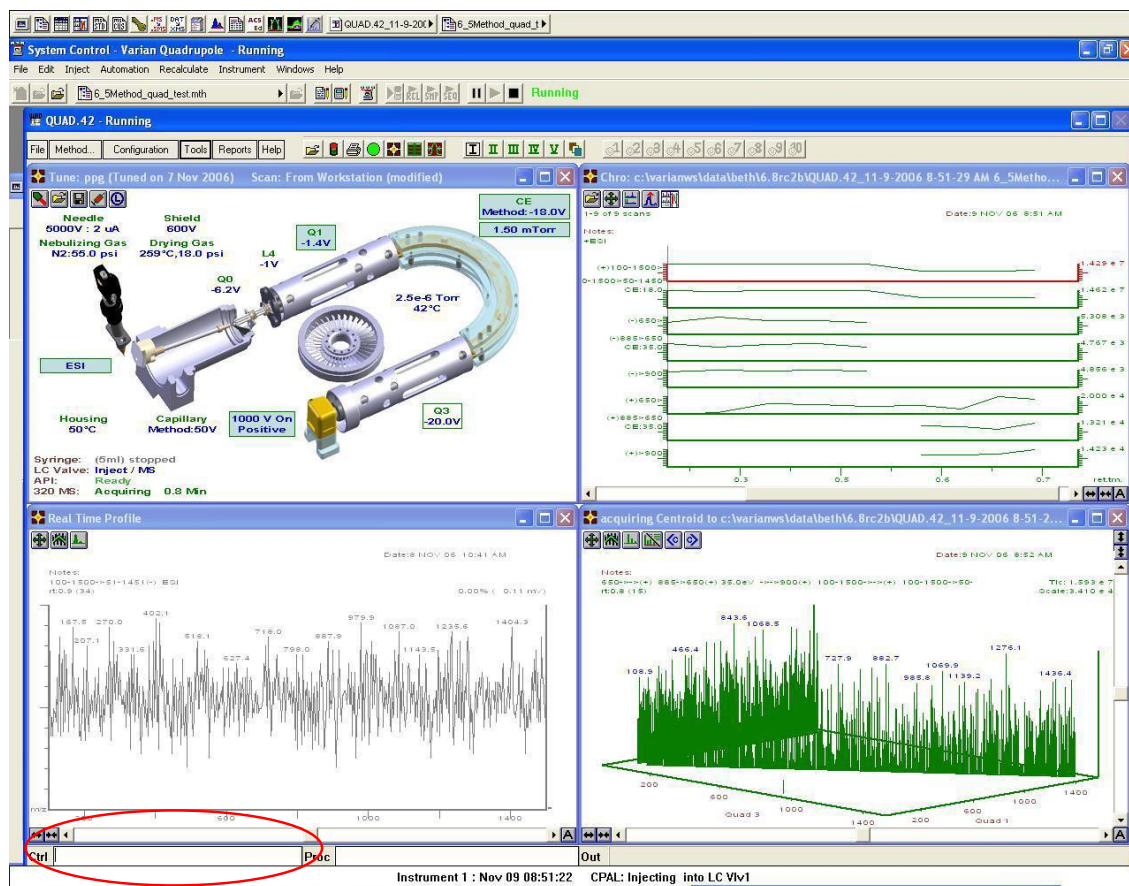
In Method Builder, open the Acquisition Method. Enable Use delay and enter the delay time in minutes.



MS/MS Breakdown

The Breakdown Curve makes MS/MS method development easy. The sample is introduced into the mass spectrometer API source with a syringe pump. A precursor ion is selected for MS/MS breakdown curves.

The precursor ion can be viewed in the profile or centroid mode by entering SW xxx in the Ctrl text field, where xxx is the desired mass.



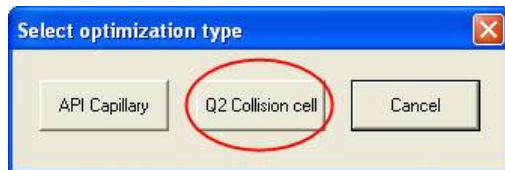
To create a Breakdown Curve, do the following:

1. On the **Tools** menu, click **MS/MS Breakdown**.



- In GC/MS mode, your only choice is Q2 collision cell.
- In LC/MS mode, you can select Q2 Collision Cell Breakdown, or API Capillary Breakdown.

2. Click **Q2 Collision cell**.



The **Create a breakdown curve** window opens.

1. Enter the precursor ion in Parent mass.
2. Click **Turn on CID gas**. Wait about a minute for it to stabilize.
3. Select either **Normal** (0.5 V steps) or **Fast** (2V step) Collection speed. Either is adequate for most conditions.
4. To save the data to a method, select **Enable**, select **Save**, choose the number of products to save.
5. Click **Browse** to select the method in which to save the product ions with the highest intensities.
6. Select **Apply**, and then **Start**.

Create a breakdown curve

This function is used to optimize the collision energy for a given parent mass. It will generate and plot the relative intensity of the product ions vs. Q2 collision energy. (in real time, use the 'opt_cid' PML)

Parent mass:

☐ Include parent -> parent in breakdown curves

☐ Auto find product masses from mass to

☒ Use these product masses

Mass 1:
 Mass 2:
 Mass 3:
 Mass 4:
 Mass 5:

Collection speed:
☐ Fast
☒ Normal

Graph scale:
☒ Absolute
☐ Scale each trace

Smooth curves:
☒ Smooth
 Points

Add ions to scan method:
☒ Enable
☐ Save highest ions to method
☒ Append
 Method folder: C:\Varian\WS\Examples\1200 MS Data Files\

☐ Turn off syringe pump after collecting breakdown curves

The breakdown curves are displayed.

To add additional ions to the method, repeat the process for the next precursor ion. For example, type **SW 790** in the Ctrl line (or SW and whatever precursor ion you choose).

For this additional precursor ion, select **Auto find product masses** or specify the product masses.

To add ions and collision voltages to an existing method, select **Append** and the appropriate method.

One option is to create a breakdown curve by scanning the API capillary.

To create a breakdown curve by scanning the API capillary, do the following:

1. Click **Create a breakdown cure by scanning the API capillary**.
2. Enter a range to auto find product masses or enter up to five masses.
3. Select either **Normal** (0.5 V steps) or **Fast** (2V step) Collection speed. Either is adequate for most conditions.
4. To save the product ions to a method, select **Enable**, select **Save**, choose the number of products to save.
5. Click **Browse** to select the method in which to save the product ions with the highest intensities.
6. Select **Apply**, and then **Start**.

Create a breakdown curve by scanning the API capillary

This function is used to optimize the API capillary. It will generate and plot the relative intensity of the product ions vs. capillary voltage.

☐ Auto find product masses from mass to

☒ Use these masses

Mass 1
 Mass 2
 Mass 3
 Mass 4
 Mass 5

Collection speed: ☐ Fast ☒ Normal

Graph scale: ☒ Absolute ☐ Scale each trace

Smooth curves: ☒ Smooth Points

Add ions to scan method: ☒ Enable

☐ Save highest ions to method

☒ Append

Method folder: C:\Varian\WS\Examples\1200 MS Data Files\

☐ Turn off syringe pump after collecting breakdown curves

The breakdown curves are displayed.

To add additional ions to the method, repeat the process for the next precursor ion. For example, type **SW 790** in the Ctrl line (or SW and whatever precursor ion you choose).

For this additional precursor ion, select **Auto find product masses** or specify the product masses.

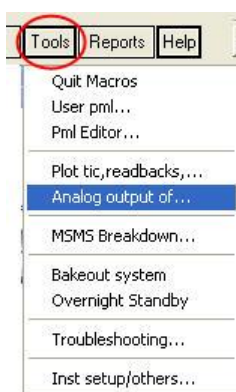
To add ions and collision voltages to an existing method, select **Append** and the appropriate method.

Analog Channels

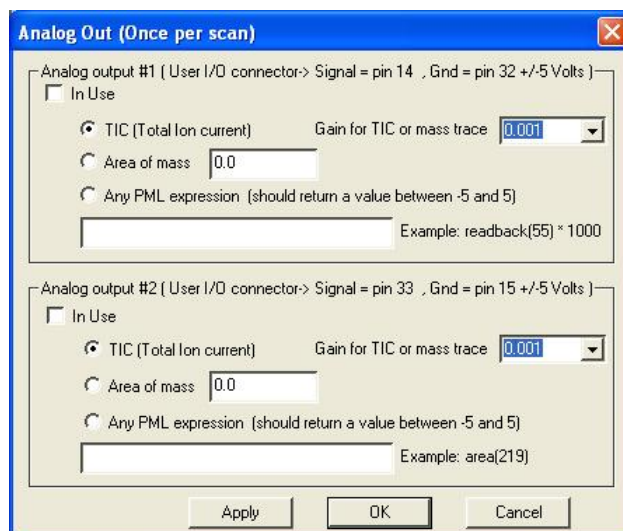
Two analog channels can be configured in the 300 Series using Analog Out selections or by defining PML outputs.

To use Analog Out, do the following:

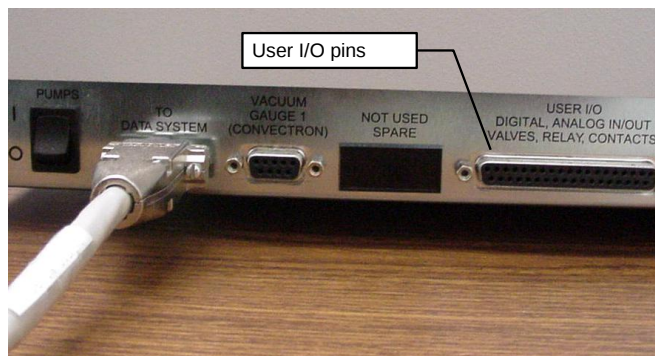
1. Select **Analog output of...** from the Tools Menu



2. The **Analog Out** widow opens.



3. Connect the wires to the pins on the User I/O connector on the back of the instrument. For example, in the preceding screen Analog output #1, the signal wire, connects to pin 14 and the ground connects to pin 32.
4. Check **In Use** for the appropriate channel in the Analog Out dialog. The part number of the user I/O Board is CUB06-0047.



Automation File Editor

Overview

Use the Automation File Editor to create and edit SampleLists, RecalcLists, and SequenceLists outside of the MS Workstation System Control application. Access the off-line Automation File Editor without disrupting automated runs.

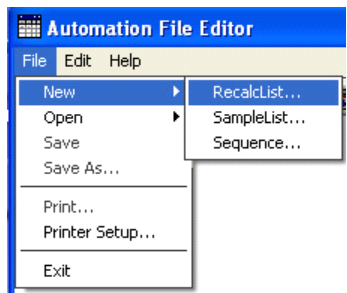
NOTE: SampleLists and Sequences that are active and running in System Control cannot be accessed in the off-line Automation File Editor.

Accessing the Automation File Editor

Click the **Automation File Editor** button  on the Workstation Toolbar.

Create or Edit a RecalcList

Select a New RecalcList, or Open an existing RecalcList from the File menu.



The RecalcList window opens. The RecalcList may contain autosampler and sample specific data handling information. The RecalcList contains the Data File name and data file specific data handling information. Fields, common to both the RecalcList and the SampleList, are described in the SampleList section.

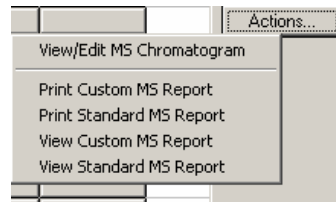
	Data File	Sample Name	Sample Type	Cal. level	Inj.	Recalc Notes	AutoLink	Amou (IS, N)	
1			New Calib Block						Add
2	c:\varianws\data\version_631\pesticide_linearity\flow_5ml\pest_2ng_5ml_1.sm Pest_2ng_5ml		Calibration	2	1	none	none		Insert
3	c:\varianws\data\version_631\pesticide_linearity\flow_5ml\pest_1ng_5ml_1.sm Pest_1ng_5ml		Calibration	3	1	none	none		Delete
4	c:\varianws\data\version_631\pesticide_linearity\flow_5ml\pest_500pg_5ml_1.: Pest_500pg_5ml		Calibration	4	1	none	none		Fill Down
5	c:\varianws\data\version_631\pesticide_linearity\flow_5ml\pest_200pg_5ml_1.: Pest_200pg_5ml		Calibration	5	1	none	none		Defaults...
6	c:\varianws\data\version_631\pesticide_linearity\flow_5ml\pest_100pg_5ml_1.: Pest_100pg_5ml		Calibration	6	1	none	none		Browse...
7	c:\varianws\data\version_631\pesticide_linearity\flow_5ml\pest_50pg_5ml_1.sr Pest_50pg_5ml		Calibration	7	1	none	none		Report...
8	c:\varianws\data\version_631\pesticide_linearity\flow_5ml\pest_20pg_5ml_1.sr Pest_20pg_5ml		Calibration	8	1	none	none		Actions...
9	c:\varianws\data\version_631\pesticide_linearity\flow_5ml\pest_10pg_5ml_1.sr Pest_10pg_5ml		Calibration	9	1	none	none		
10									
11									

Recalc Notes: Enter notes about the Recalculation of the Data File.

AutoLink: Enter post calculation operations.

Report: Generate a report for the selected data file. Note that if a data file is not highlighted in the Data File column, no report is generated.

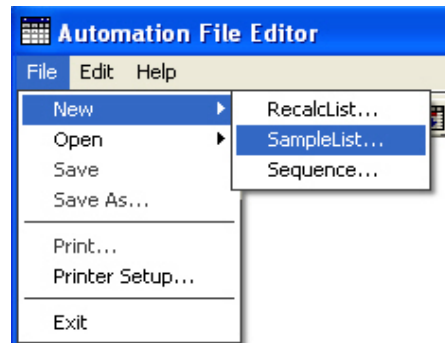
Actions: After generating a report using the Report button, click **Actions** to show the possible actions.



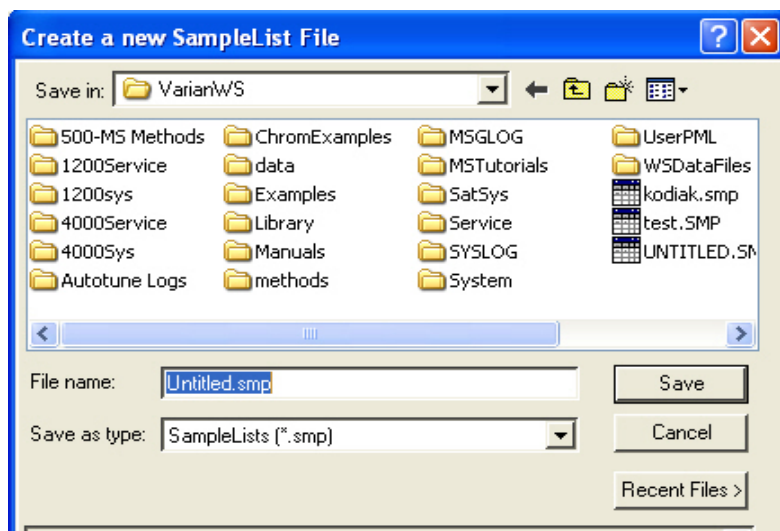
Create or Edit a SampleList

To create or edit a SampleList, do the following:

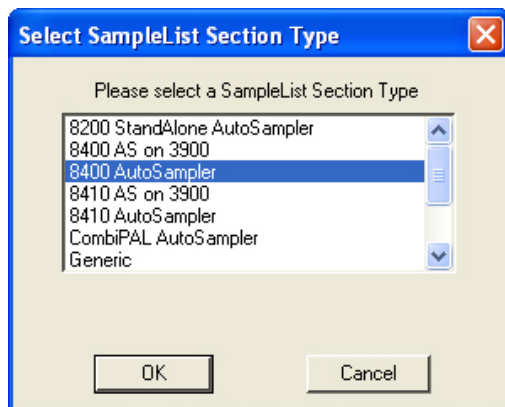
1. From the **File** menu, select **New** to create a new SampleList or select **Open** to open an existing SampleList to edit.



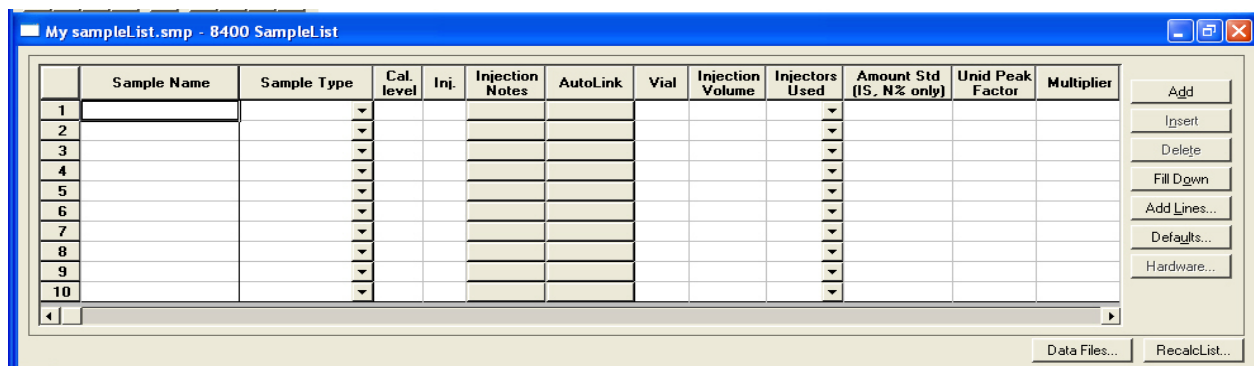
2. Select a folder for the SampleList, type a name, and click **Save**.



3. Select the autosampler and click **OK**.



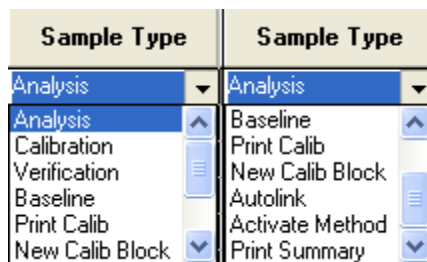
4. Size the Spreadsheet columns by dragging their borders with the left mouse button. Right-clicking a column header displays formatting options. The Sample Name column does not scroll.



SampleList Fields

Sample Name: Enter the sample name. Click **Data Files** to enter sample names. If only '%s' is listed in the Data Files, the sample name is as you entered it.

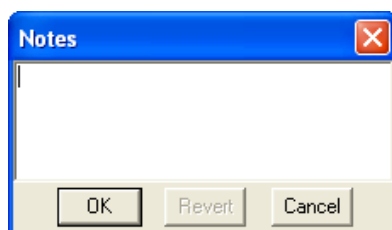
Sample Type: Use the scroll bar to see all options.



Cal. Level: Designate the calibration level for a Calibration sample. You can enter up to ten levels.

Inj: Specify the number of injections of the sample. You may make up to nine replicate injections of each sample.

Injection Notes: Enter notes about the sample.

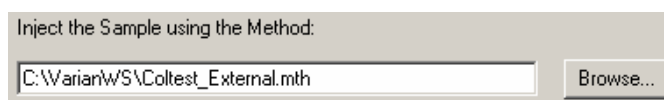


AutoLink: Refer to "Inject Single Sample Menu" on page 14.

Vial	Injection Volume	Injectors Used	Amount Std (IS, N% only)	Unid Peak Factor	Multiplier	Divisor	MultiChannel MultiStandard
0	1.0	Pos 1	1	0	1	1	none

In the Vial, Injection Volume, and Injectors Used fields, enter the appropriate information.

The field beginning with Amt. Std. is only for data files acquired with standard GC detectors.



Select the **Method** for the run. Click **Browse** to select a file.

Other Fields

Add: Adds a new line to the end of the list.

Insert: Inserts a new line before the currently active line.

Delete: Deletes the currently active line.

Fill Down: When sections of columns or entire lines are highlighted, the information in the top highlighted row is repeated to the lowest selected row.

Add Lines: Add several similar lines to the SampleList. Enter the common information in the dialog box. Fields in Add Lines may vary from one autosampler to another. Only the fields associated with the selected autosampler are displayed.

For sequentially numbered Sample names, check the box and enter the starting number and the number of entries to add to the SampleList. The Sample Names will have these numbers appended to them.

Defaults: Change the default entries in the table, such as Injection Volume, Injectors Used, etc. After defining new defaults, click **Save** to activate the new defaults.

Data Files: Change the location and name of the Data Files.

RecalcList: Click and generate automatically a RecalcList associated with single sample acquisitions.

Specifying the Data File Name and Path

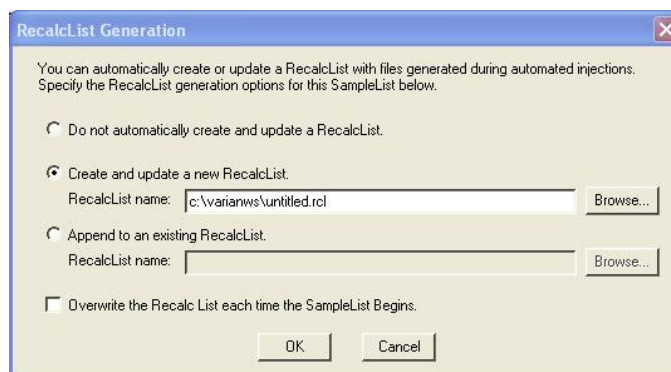
Data File names can be up to 256 characters long. Sample ID, injection date, module name, and injection number can be embedded in the file name making the Data File name correlate with each sample injection.

Click **Data File** to open the **Data Files Generation** window. Select the path and the file name for the data file.

Select the data file directory from the left side. Create a file name specification on the right. Combine text entry with the “%” variable symbols to specify file names with sample injection specific information. An example of the file name is updated as you enter the file name specification.

Specifying a RecalcList

To select the desired RecalcList option, click **RecalcList**. The RecalcList Generation window opens. You can create a new RecalcList, append to an existing RecalcList, or not create nor update a RecalcList. When you select create and update a new RecalcList, the automatically generated RecalcList does not overwrite an existing RecalcList. If a RecalcList with the same file name exists, the newly created RecalcList has a number appended to its file name to make it unique and to prevent the older RecalcList from being overwritten.



The RecalcList Generation dialog box contains the following elements:

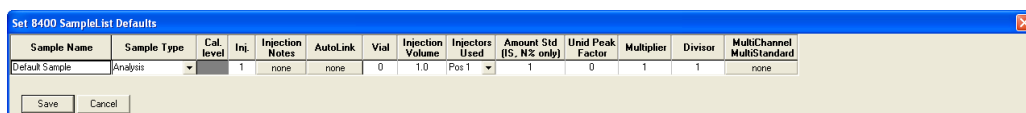
- Instructional text: "You can automatically create or update a RecalcList with files generated during automated injections. Specify the RecalcList generation options for this SampleList below."
- Three radio button options:
 - ☐ Do not automatically create and update a RecalcList.
 - ☒ Create and update a new RecalcList.
 - RecalcList name:
 - ☐ Append to an existing RecalcList.
 - RecalcList name:
- ☐ Overwrite the Recalc List each time the SampleList Begins.
- OK and Cancel buttons at the bottom.

Changing Default SampleList Entries

When you add a new row to a SampleList, default values are used for each entry.

To change the default values:

1. Click **Default** in the open SampleList window.
2. Enter the desired default values and click **Save**.



The Set 8400 SampleList Defaults dialog box displays a table of default values for a sample list entry.

Sample Name	Sample Type	Cal. level	Inj.	Injection Notes	AutoLink	Vial	Injection Volume	Injectors Used	Amount Std (IS, N2 only)	Unit Peak Factor	Multiplier	Divisor	MultiChannel MultiStandard
Default Sample	Analysis		1	none	none	0	1.0	Pos 1	1	0	1	1	none

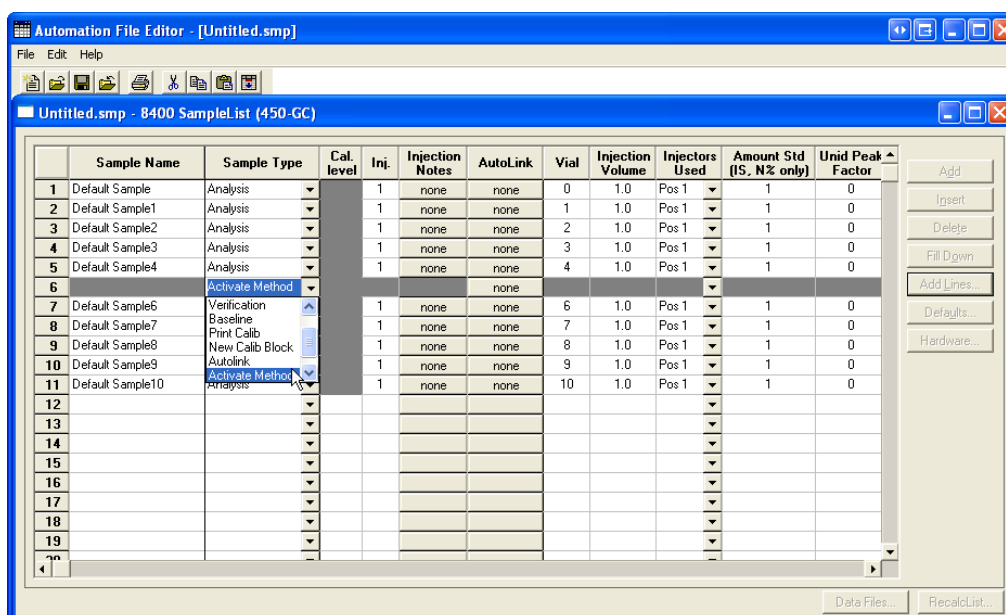
Save Cancel

Using More Than One Method for Injections

You can do automated injections using more than one Method by changing the active Method from the SampleList or using a Sequence.

Changing the Method in the SampleList

Change the Method used during injections by activating a Method in a SampleList row.



Select **Activate Method** from the Sample Type cell.

Click **AutoLink** in the row that you are working.

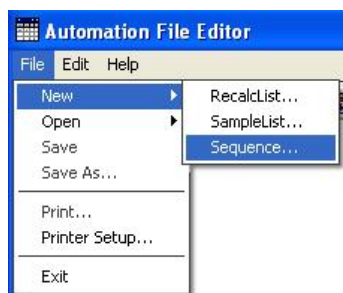
Enter the name of the Method or click **Browse** to select the Method from a list.

Specify any number of Methods in the SampleList.

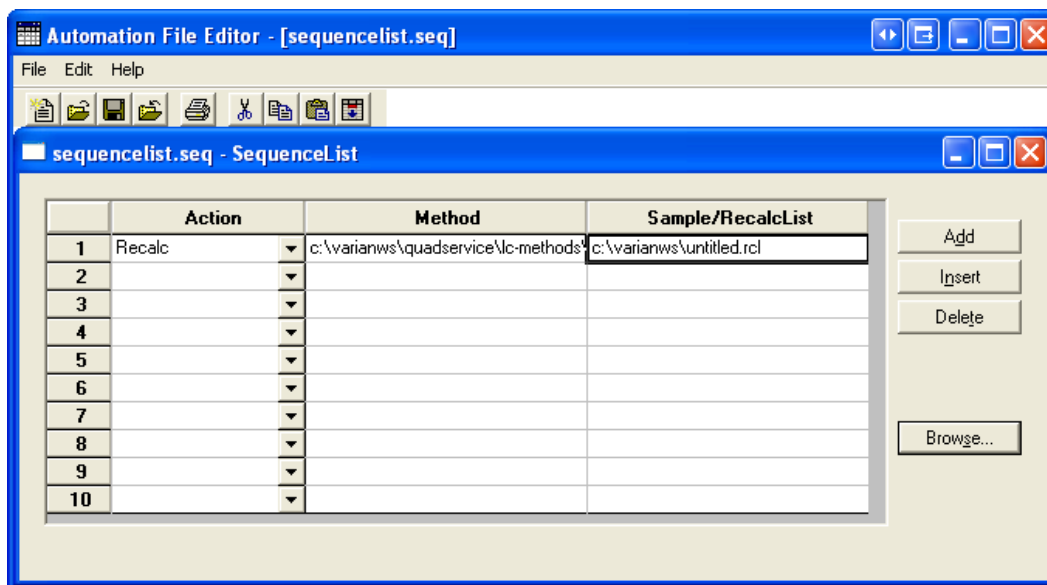
Create or Edit a Sequence

To create or edit a sequence do the following:

1. From the **File** menu select **New** and then **Sequence** or select **Open** and then **Sequence** from the File menu.



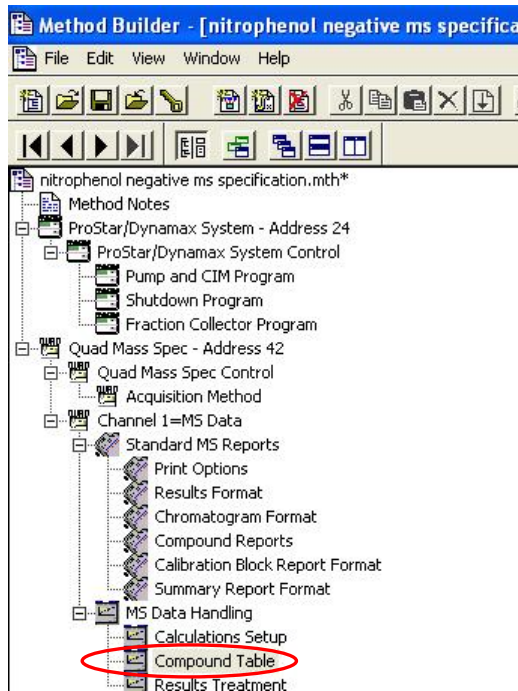
2. Click **Add** to add lines to the SequenceList.
3. Enter the required number of Sequence lines.
4. Select the **Action** for the selected step.
5. Click **Browse** to select the Method and SampleList files.



Compound Table

Use Compound Table for automatic quantitation with external or internal standards. The Compound Table is part of the data handling method. In the Method Builder tree, click **Compound Table** under MS Data Handling.

Click **Show/Hide Directory** to display the method full screen.



Creating a Compound Table

1. Click **Compound Table**.
2. Click **Select Data File**, click the data file of your choice, and click **Open File**. This data file becomes the Reference Data File.
3. Click **Build Compound List** to open the data file in MS Data Review.
4. Click the apex of the desired peak in the chromatogram to generate a spectra and place information in the Spectrum List.
5. Close MS Data Review.
6. Click **Import Compound List**, and click the spectra from the table and then click **Select**.

The compound is added to the Compound List.

NOTE: Double-click a cell to display more information.

	RT	IS	Compound ID	Quan Ion	Calculations	Integration	Identification	Ref. Spectrum
1	6.491		Benzene, 1,3-dimethyl	133.9, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	133.9, 77.0, 78.9
2	7.385		Hexachlorocyclopentadiene	236.9, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	236.9, 203.0, 207.0
3	8.209		Benzene, 2-methyl-	165.0, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	165.0, 63.0, 147.0
4	8.493	X	Acenaphthene-d10	162.2, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	162.2, 164.1, 166.1
5	8.209		Benzene, 1-methyl-	165.0, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	165.0, 118.9, 89.9
6	9.447		Benzene, 2,4-dimethyl	120.0, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	120.0, 176.0, 168.0
7	10.650		Benzene, hexachloro-	284.0, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	284.0, 286.0, 288.0
8	10.965		Simazine	201.0, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	201.0, 186.0, 177.0
9	11.054		Atrazine	200.0, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	200.0, 215.0, 207.0
10	11.393		Lindane	183.0, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	183.0, 181.0, 211.0
11	11.756	X	Anthracene-D10	188.1, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	188.1, 189.1, 187.1
12	13.087		Metribuzin	197.9, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	197.9, 199.0, 144.0
13	13.255		Alachlor	188.0, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	188.0, 160.1, 141.0
14	13.545		Heptachlor	272.0, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	272.0, 100.0, 271.0
15	14.602		Metolachlor	162.1, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	162.1, 238.0, 241.0
16	14.946		Cyanazine	225.0, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	225.0, 198.0, 177.0
17	14.947		Aldrin	212.2, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	212.2, 263.0, 66.0
18	16.384		Heptachlor epoxide	352.9, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	352.9, 354.9, 356.9
19	17.382		cis-Chlordane	375.0, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	375.0, 373.1, 371.1
20	17.755		Butachlor	176.2, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	176.2, 160.2, 188.0
21	17.956		trans-Chlordane	375.0, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	375.0, 373.0, 371.0
22	18.069		trans-Nonachlor	409.0, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	409.0, 406.9, 411.0
23	19.208		Dieldrin	79.0, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20	0.20, Spec	79.0, 81.0, 276.9

Reference Data File: Select Data File

Build Compound List Import Compound List Export Compound List Print...

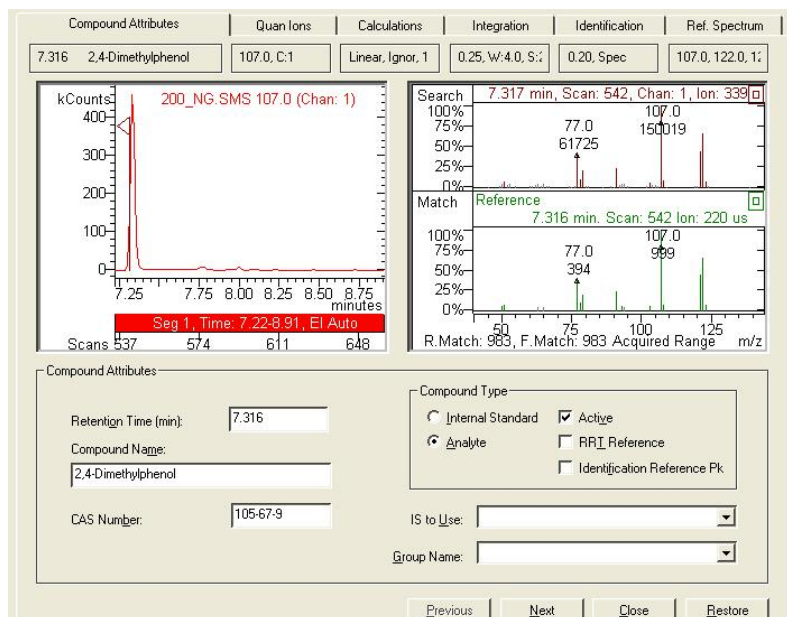
View Curves Sort Add Insert Delete Fill Down Restore

The Compound table has the following fields; Retention time (Ret), Internal Standard (IS), Compound ID, Quantitation Ion (Quan Ion), Calculations, Integration, Identification, and Reference Spectrum (Ref Spectrum).

- Click **Select Data File** to open a data file.
- Sort, Add, Insert, Delete, Fill Down, or Restore compounds.
- Other functions are: Build Compound List, Import Compound List, Export Compound List, and Print.
- Before processing calibration files, review the compound table to check that the entries are correct.
- Double-click a cell to open the **Compound Tab** view. In this example, Ret 7.316 was selected.

Compound Attributes

The following shows the **Compound Attributes** tab view after the retention time 7.613 was double-clicked. The Chromatogram and Spectrum Displays are on top and the bottom part has fields. Add information, such as Compound Name and CAS Number, during the peak addition process.



Edit Name, CAS Number, Retention Time

Edit the Compound Name and CAS fields to describe your compound

Click the chromatogram display to update the Retention Time. The spectrum of the selected scan is displayed. It becomes the new reference spectrum if you select it when you exit the tab dialog, or click **Next**, or **Previous** to move to a different entry.

Identify Internal Standards

By default, compounds are identified as Analytes. Identify all Internal Standards by selecting the **Internal Standard** option button in the Compound Type section, as in previous screen shot. Click **Next**, or **Previous** to check the Compound ID information of the other analytes. If more than one internal standard is identified, select the internal standard for a particular target compound from the IS to Use list.

Identify Group Members

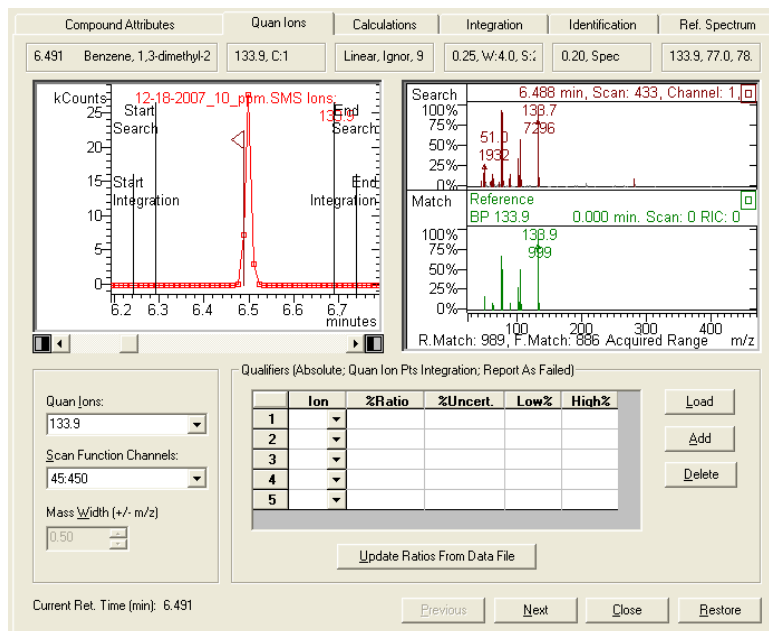
Sometimes target compounds are identified as a member of a group of compounds (for example, Trihalomethanes (THM), alkyl aromatics, etc.).

Enter the desired name in the Group Names field.

If more than one Group is designated in a method, select the Group Name from the list.

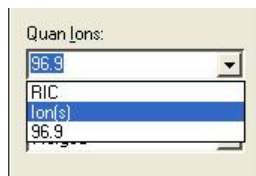
Quan Ions

Click the **Quan Ions** tab in the Compound Table editor. When peaks are added to the Compound Table, the software names the Base Peak (most intense ion) the Quantitation Ion. The plot shows the mass chromatogram for the chosen Quan Ion.



Edit Quan Ions

Select a different Quan ion, a sum of ions, or a range of ions.



If you selected Ion(s), Select Ions to Plot opens. Select Show Format and Examples to display the ways to specify ions. The Plot is redrawn automatically after you select the Quan Ions. You can determine if the chosen Quan ions integrate cleanly or if there are interferences due to co-eluting peaks or background contamination.

NOTE: The Scan Function Channels field is only relevant for MS/MS or SIM analysis, because quantitation is done only on individual Channels of information.

Select Ions to Plot

Edit Ion Formula
The valid ion range is from 2.0 to 2000.0. STATUS: Valid Ion Formula
IONS: RIC

☒ Show Format and Examples

Format and Examples
Specify an ion selection by combining one or more of the following items, with the '+' and '-' operators.
- Individual Ions (e.g., 40.0)
- Range of ions (e.g., 40.0:60.0)
- All ions: RIC
Examples: 28.0 (Plot ion 28.0 only.)
40.0:450.0 (Plot ions 40.0 through 450.0.)
RIC-128.0 (Plot all ions except ion 128.0.)
91.0+128.0 (Plot ions 91.0 and 128.0.)
60.0:450.0-128.0 (Plot ions 60.0 through 450.0 except ion 128.0.)

Help OK Cancel

Edit Retention Time

To change the retention time, click the desired scan in the Chromatogram display.

Look at Other Compounds

Click **Next**, or **Previous** to see the Quan Ion information for other peaks in the Compound Table.

Select Qualifier Ions

In addition to specifying quantitation ions, you can select qualifier ions. Click **Load** to enter automatically the three most intense qualifier ion candidates present in the Reference Spectrum.

Qualifiers (Absolute; Quan Ion Pts Integration; Report As Failed)

	Ion	%Ratio	%Uncert.	Low%	High%
1	77.0	105.5	20.0	85.5	125.5
2	78.9	97.7	20.0	77.7	117.7
3	106.0	52.3	20.0	32.3	72.3
4					
5					

Load Add Delete

Update Ratios From Data File

Click **Add** to add the next most intense reference spectrum ion.

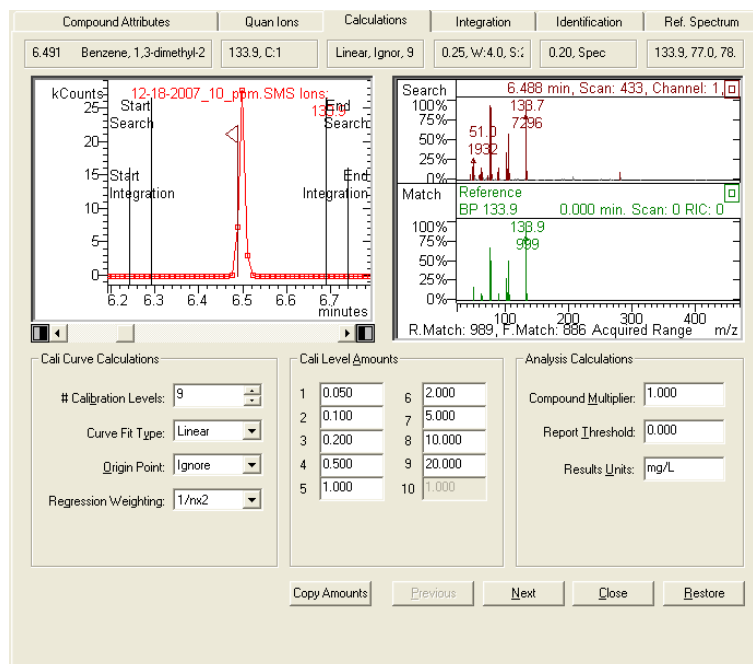
The Qualifiers Table has the following fields:

- **Ion:** Click in the Ion field to see the choices.
- **Ratio:** Shows the intensity of the qualifier ion as a percentage of the chosen Quan ion(s).
- **%Uncert.:** Allowed percentage deviation from the Ratio. You can change the default of 20%. The % Uncertainty allowable range depends on the Ion Ratio Type setting in the Calculations Setup Dialog (Absolute % or Relative %).
- **Low% and High%:** For ion 63, the top line in the previous example and the allowed range for the ratio is $87.5.0 \pm 20\%$ (absolute). Therefore 67.5% is the Low% value and 107.5% is the High% value area.

As samples are processed (Calibration, Analysis, or Verification runs), the Qualifier Ion tests are done before the peak is integrated.

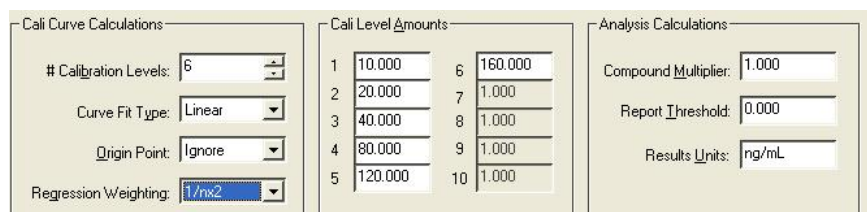
Calculations Tab

Click the **Calculations** tab to display the following.



Enter Number of Calibration Levels and Amounts

Enter the number of calibration levels, information about the calibration curve, the calibration amounts, and results units.



The Calculations Information is updated in the Compound Table. This information can be automatically entered for the other compounds in the table.

Quan Ion	Calculations	Integration
133.9, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20
236.9, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20
165.0, C:1	Linear, Ignor, 9	0.25, W:4.0, S:20

Click **Copy Amounts** to automatically enter the first value for the other levels. Repeat this process for all standards in the Compound Table.

Select Curve Fit

Select the desired curve fit from the list.

The screenshot shows a dialog box titled "Cali Curve Calculations". It contains three main settings:

- "# Calibration Levels": A numeric input field with the value "1".
- "Curve Fit Type": A dropdown menu currently showing "Linear".
- "Origin Point": A dropdown menu with a list of options: "Linear", "Quadratic", and "Cubic". The "Linear" option is currently selected.

For most calibration curves, use either Linear or Quadratic.

NOTE: For more information about the Integration, Identification, and Reference Spectrum Tabs, and other information about Quantitation and Data Handling: see the *MS Software Reference Manual*, part number 391496300.

Security Administration

Overview

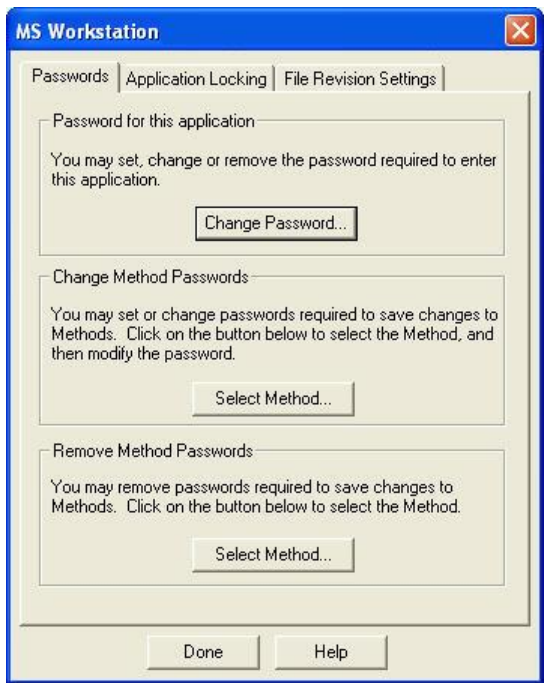
The Security Administration window contains three categories of security parameters. These features are tools for compiling with 21CFR part 11.

- Passwords
- Application Locking
- File Revision Settings

Click the **Security** button on the Workstation Toolbar to open the Security Administration window.



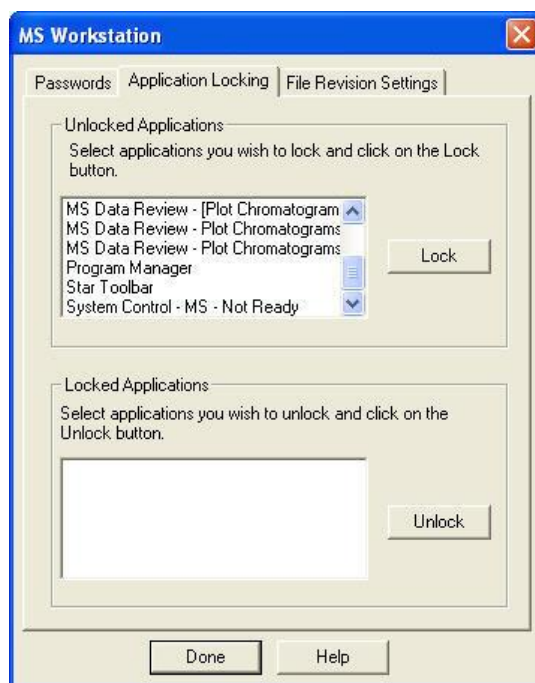
Passwords



Area	Description
Password for this application	Specify a password required to open the Security Administration application. NOTE: There is no way to recover this password if it is lost, so document the password in a secure location.

Area	Description
Change Method Passwords	Method passwords can be added, changed, and removed from the Security Administration application. Click Select Method to browse for and select the desired Method. After the Method is selected, you are prompted either for a new password (if no previous password exists for the Method), or for the old and new password (if the Method already contains a password). NOTE: that if creation of new passwords is disabled in the File Revision tab, you cannot add a new password to a Method that does not already contain one. Change or add Method passwords in the Method Builder and Interactive Graphics applications.
Remove Method Passwords	Security Administrators can remove Method passwords without entering the existing password. This is useful if the password for a Method was lost. Click Select Method, select the desired Method, and the password is removed.

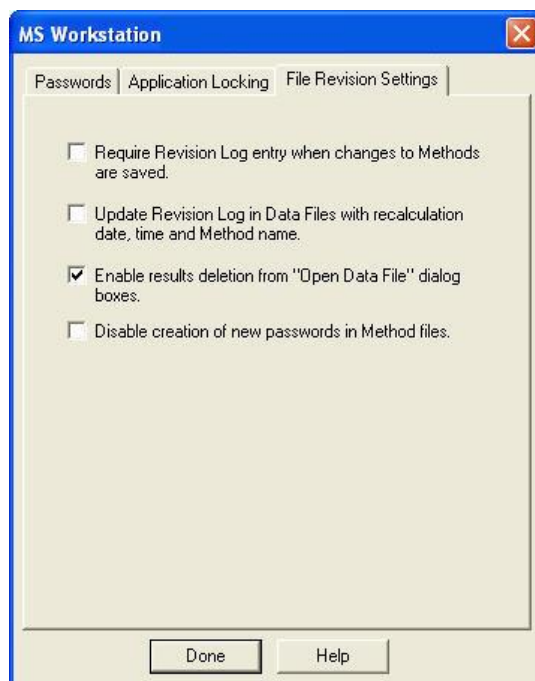
Application Locking



Area	Description
Unlocked Applications	Lists the top-level windows currently running and not locked. Select any number of them and click Lock. They move to the Locked Applications list and their windows are disabled (they will not respond to mouse or keyboard input). Note applications locked by the Security Administration stay locked after the Security Administration application closes.

Area	Description
Locked Applications	Lists the top-level windows currently running and locked. Select any number of them and click Unlock. They move to the Unlocked Applications list and their windows are enabled (they respond to mouse or keyboard input).

File Revision Settings



Area	Description
Require Revision Log entry when changes to Methods are saved.	When checked, prompts you for a description of changes when a Method file is altered and saved. The Revision Log appears: - Listed in the Notes of the File Open dialog box. - Listed in the Method Builder application window when the Method is open. - Included in the Method printout.
Update Revision Log in Data Files with Recalculation date, time, and Method name.	Data Files are updated with a time stamp and Method name when they are recalculated (either from System Control or from Interactive Graphics). The Log can be included in printed reports.
Enable results deletion from "Open Data File" dialog boxes.	A button appears in the Open Data File dialog allowing results to be deleted from a specified channel of a Data File. Results deletions are logged in the Data File's Revision Log. This option only affects standard GC results. GC/MS results will not be deleted.

Area	Description
Disable creation of new passwords in Method files.	When checked, new passwords cannot be added to Methods. Methods with passwords prompt users for their password before saving changes.

Configuring HPLC Modules

Overview

The Varian MS Workstation supports the Varian HPLC modules and the HTS PAL.

Refer to the 212-LC Operation Manual, part number, 395410300 for more information.

Configuring GC Modules

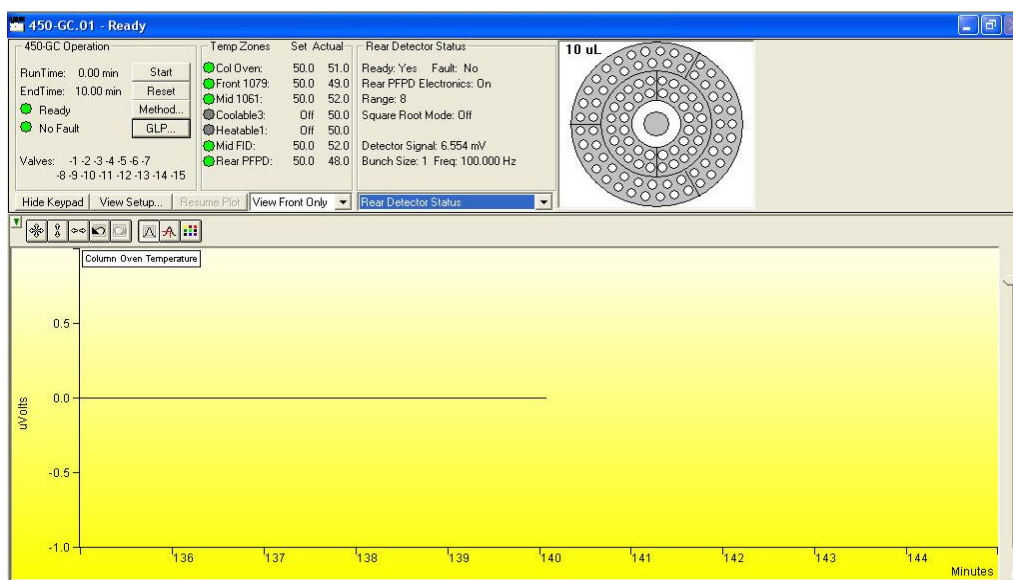
Overview

Since the 400 Series GC communicates with the Workstation over a standard Ethernet connection, your system can easily be expanded from a single 400 Series GC/single Workstation configuration, to multiple GC/Workstations, to a fully networked lab with a virtually unlimited number of GCs and Workstations. Ethernet refers to the cables and interface cards that connect devices to the network. If you are connecting your GC to an existing Ethernet network, you need to know which type of cable to use. Refer to the *Communications* section of your GC Operator's Manual.

The 400 Series GCs uses TCP/IP (Transmission Control Protocol / Internet Protocol) to communicate over the Ethernet network. The Workstation PC and each GC needs a unique IP address—the addresses that are used to identify each networked TCP/IP device.

450-GC System Control Command Reference

Status and Control Window



The 450-GC Status and Control window has five display areas; the 450-GC Operation display, the Temperature. Zones Status display, the Component Status display, the 8400/8410 Carousel display, and the Chromatogram display.

The left-most display area is the 450-GC Operation display, which contains information about the current run and the overall state of the GC.

The display area to the right of the 450-GC is the Temperature Zones Status display, which shows the setpoint and current actual temperature of each heated zone in the GC.

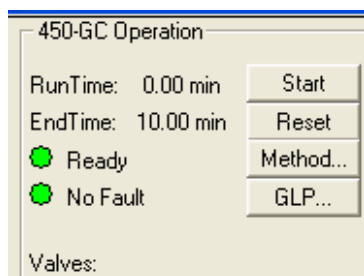
Next is the Component Status display. Select the component for which you wish to see more detailed status information, including ready and fault status for the selected component. You can change the component being displayed using the selection box below the display area, or by clicking on the corresponding temperature zone entry in the temperature zone status display.

450-GCs that have an 8400 AutoSampler or 8410 AutoInjector installed will have another display area, the 8400/8410 Carousel display, that shows a graphical representation of the 8400 or 8410 Carousel. This display graphically shows, which vials are to be sampled, which vials have been sampled, which vial is currently being sampled.

Below these display areas is the Chromatogram display. A selection box above the chromatogram allows you to select the channels for which you want to view the real-time chromatogram.

450-GC Operation Display

The 450-GC Operation display is in the left portion of the 450-GC Status and Control window.



Item	Description
Run Time	Show the elapsed time in minutes since the beginning of the run. The maximum run time is 999.99 minutes.
End Time	Show the time the run ends.
State	Ready, Running, Stabilizing, Equilibrating, Computing, Needs Monitor, Monitoring, Sampling, Connecting, or Not Ready Show the state of the GC. The light appears green if the GC is Ready or Running. Otherwise, the light is red.
Fault/No Fault indicator	No Fault (green light) or Fault (red light). When a hazardous or disabling fault occurs, any run in progress will halt and the affected component will shut down. If the fault is recoverable, then the run is not terminated.
Valves	Display the 450-GC valve status. A plus sign (+) precedes the valve number if its state is energized. A minus sign (-) precedes the valve number if the valve is in the default state or if the valve is unused.
Start	If the system is Ready, start the GC Method and sends a start signal to the GC. Equivalent to pressing Start on the front panel of the GC. The Start button is disabled unless the 450-GC is in the Ready state.
Reset	Reset the GC, advancing it to the next state. If RUNNING, the GC aborts the current run, goes to the READY state, and continues with the next injection in the Sequence. Equivalent to pressing Stop on the front panel of the GC.
Method	Open the Method Builder application for editing the active 450-GC method.
GLP	Display information about the IP address, the current revisions of the interface library and GC driver, the main board, the keypad, the IOC, the IOE and the number of strokes on the A/S plunger.

Temperature Zones Status Display

Temp Zones	Set	Actual
● Col Oven:	50.0	51.0
● Front 1079:	50.0	49.0
● Mid 1061:	50.0	52.0
● Coolable3:	Off	50.0
● Heatable1:	Off	50.0
● Mid FID:	50.0	52.0
● Rear PFPD:	50.0	48.0

The temperature zones are displayed in the middle of the 450-GC Status and Control window. The display includes the setpoints and actual temperatures of the column oven, the three zones that can be cooled and heated, and the three zones that can only be heated. The display is **Fault**, if a fault occurs, and **Off** if the zone oven is off. If the zone has not been configured by the 450-GC, then **N/A** is displayed for the setpoints and actual temperature. Clicking one of the temperature zone entries displays the corresponding component status in the Component Status Display.

The LEDs indicate the status of each temperature zone. If the zone is not configured or the zone oven is off, the LED is gray. If the temperature zone is Not Ready or there is a fault, then the LED is red. Otherwise, the LED is green.

Component Status Display

The Component Status display is in the right portion of the 450-GC Status and Control window. Select the component from the drop down box.

Front Injector Status

Ready: Yes Fault: No
1079 Oven: On Coolant: On
Setpoint: 50.0 C Actual: 49.0 C
Split State: On Split Ratio: 50

Enable 1079 Injector Coolant at 250.0 C
Timeout: 20.00 min Timed Out: No

Front Injector Status

Column Oven Status

Column Oven Status

Ready: Yes Fault: No
Oven Power: On Coolant: On
Setpoint: 50.0 C Actual: 51.0 C
Stabilization Time 2.00 min

Enable Column Oven Coolant at 50.0 C
Timeout: 20.00 min Timed Out: No

Column Oven Status

Item	Description
Ready	Yes or No The column oven is Ready (Yes) if the setpoints were reached and stable.
Fault	Yes or No Displayed if a fault in the column oven component has occurred.
Oven Power	On or Off Displays if the column oven is turned off or on.
Coolant	On or Off Displays if the column oven coolant is enabled in the active method.
Setpoint	-99 to 450 °C Displays the column oven programmed temperature setting in the active method.
Actual	-99 to 450 °C Displays the actual temperature of the column oven.
Stabilization Time	0.00 to 10.00 min Displays the 450-GC column oven stabilization time in minutes. The stabilization time counts down from the programmed method value and then displays 0.00 minutes when the stabilization period is over.
Enable Column Oven Coolant at	30 °C to 450 °C Displays the programmed column oven temperature.
Timeout	0.01 min to 999.99 min Displays the programmed coolant time-out value.
Timed Out	Yes or No Displays Yes if the coolant time-out period has elapsed.

AutoSampler Status

This option is only shown on 450-GCs that have an 8400 AutoSampler or 8410 AutoInjector connected to them.

Item	Description
8400/8410 State	Ready or Running
Current Vial	0 through 99 for 8400 AutoSampler 1 through 21 for 8410 AutoInjector
Plunger Strokes	Shows the number of times that the syringe plunger has been stroked up and down. This can be used to help monitor syringe wear and plan for syringe replacements.
Injection Mode	Shows the injection mode specified in the active 450-GC method.
Injection number: x of y	x and y are any number between 1 and 9. Shows the number of the injection that is currently being run and the total number of injections scheduled for that sample.
Injectors used	Pos 1 Pos 2 Pos 1 then 2 Pos 2 then 1 Shows the injector positions that the 8400/8410 will use for current run.
2nd Injection	Duplicate or Advance This field is only displayed when the 8400/8410 is in Dual Mode or Duplicate Mode.
Tray Orientation (8410 AutoInjector Only)	Vials 1 through 10 Vials 11 through 16 or Vials 17 through 21 Shows the range of vials accessible from the current 8410 carousel location.

Sample Delivery Status

Item	Description		
Valve 1 through Valve 7	If the valves are configured in the 450-GC, displays the assigned valve name and current state at the 450-GC. The possible valve names, default state of the valve, and the energized state of the valve are listed.		
	Name	Default State	Energized State
	Unused	Off	On
	Front Split	On (split)	Off (splitless)
	Middle Split	On (split)	Off (splitless)
	Rear Split	On (split)	Off (splitless)
	Gas Sampling	Fill	Inject
	Liquid Sampling	Fill	Inject
	Sample	Off	On
	Internal Std	Off	On
	Surrogate Std	Off	On
	Series Bypass	Series	Bypass
	Backflush to Detector	Forward	Backflush
	Backflush to vent	Forward	Backflush
	Column Selection	Column 1	Column 2
	Injection to detector	Backflush	Inject
	Injection to vent	Backflush	Inject
	Alternate injection	Column 1	Column 2
	Simultaneous Injection	Fill	Inject
	Methanizer Bypass	Series	Bypass
	Sample Preconcentration Trap	SPT Desorb	SPT Trap
	External Event A	Off	On
	External Event B	Off	On
	External Event C	Off	On
	External Event D	Off	On

1177 Injector Status

Item	Description
Ready	Yes or No The 1177 injector oven is Ready (Yes) if the setpoints have been achieved and stabilized.
Fault	Yes or No Displays if a fault in the 1177 injector component has occurred.
1177 Oven	On or Off Displays if the 1177 injector oven component is turned off or on at the 450-GC. The 1177 injector is an isothermal injector.
Setpoint	50 to 450 °C Displays the 1177 injector oven programmed temperature setting in the active method.
Actual	50 to 450 °C Displays the actual temperature of the 1177 injector oven at the 450-GC.
Split State	On or Off Displays the current split state of the 1177 injector method.
Split Ratio	1 to 10000 or Off Displays the current split ratio of the 1177 injector method. The split ratio is defined as the (Column Flow + the Split Flow) / the Column Flow.

1079 Injector Status

Item	Description
Ready	Yes or No Ready (Yes) after the setpoints are reached and stable.
Fault	Yes or No Displays if a fault in the 1079 injector component has occurred.
1079 Oven	On or Off Displays if the 1079 injector oven component is turned off or on at the 450-GC.
Coolant	On or Off Displays if the 1079 injector oven coolant is enabled in the active method.
Setpoint	-99 to 450 °C Displays the 1079 injector oven programmed temperature setting in the active method.
Actual	-99 to 450 °C Displays the actual temperature of the 1079 injector oven at the 450-GC.
Split State	On or Off Displays the current split state of the 1079 injector method.
Split Ratio	1 to 10000 or Off Display the current split ratio. The split ratio is defined as the (Column Flow + the Split Flow) / the Column Flow.
Enable 1079 Injector Coolant at	30 °C to 450 °C Display the temperature at which the coolant is enabled.

Item	Description
Timeout	0.01 min to 999.99 min Display the programmed time-out value in the active method.
Timed Out	Yes or No Displays Yes if the coolant time-out period has elapsed for the 1079 injector oven.

1041/1061 Injector Status

Item	Description
Ready	Yes or No Ready (Yes) after the setpoints are reached and stabile.
Fault	Yes or No Displayed if a fault has occurred.
1041/1061 Oven	On or Off Displayed if the injector oven is turned off or on at the 450-GC. The 1041 and 1061 injectors are isothermal injectors.
Setpoint	50 to 450 °C Displays the 1injector oven programmed temperature setting in the active method.
Actual	50 to 450 °C Displays the actual temperature of the oven.

SPT Injector Status

Item	Description
Ready	Yes or No Ready (Yes) after the setpoints are reached and stabile.
Fault	Yes or No Displayed if a fault has occurred.
SPT Oven	On or Off. Displayed if the oven component is turned off or on at the 450-GC.
Coolant	On or Off. Displayed if the oven coolant is enabled in the active method.
Setpoint	-99 to 450 °C Display the oven programmed temperature setting in the active method.
Actual	-99 to 450 °C Display the actual temperature of the oven in the 450-GC.
Enable SPT Coolant at	30 °C to 450 °C Display the programmed injector oven temperature at which the oven coolant is enabled.
Timeout	0.01 min to 999.99 min Display the programmed coolant time-out value in the active method for the oven.
Timed Out	Yes or No Yes displayed if the coolant time-out period has elapsed for the oven.

Type 21 and 25 Injector EFC Flow/Pressure Status

Item	Description
Ready	Yes or No Ready (Yes) after the setpoints are reached and stable.
Fault	Yes or No Displayed if a fault has occurred.
Pressure Setpoint	0.1 to 150 psi Display the column head pressure setting in the method.
Actual Pressure	0.1 to 100 psi Display the actual column head pressure at the 450-GC.
Column Flow	Display, in mL/min, the column flow rate calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).
Linear Velocity	Display, in cm/sec, the column linear velocity calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).
Total Flow	Display, in mL/min, the total flow rate through the system.
Split State	On or Off Display the current split state of the 1079/1177 injector method.
Split Ratio	1 to 10000 Display the current split ratio of the 1079/1177 injector method. The split ratio is defined as the (Column Flow + the Split Flow) / the Column Flow.

Type 23 Injector EFC Flow/Pressure Status

Item	Description
Ready	Yes or No Ready (Yes) after the setpoints are reached and stable.
Fault	Yes or No Displayed if a fault has occurred.
Flow Setpoint	0.1 to 50 mL/min Display the programmed column flow rate setting in the active method.
Actual Flow	0.1 to 50 mL/min Display the actual column flow rate calculated from the measured head pressure and column parameters (carrier gas, column length, and internal diameter).
Pressure	Display, in psi, the measured column head pressure.
Linear Velocity	Display, in cm/sec, the column linear velocity calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

Type 24 Injector EFC Flow/Pressure Status

Item	Description
Ready	Yes or No Ready (Yes) after the setpoints are reached and stable.
Fault	Yes or No Displayed if a fault has occurred.
Pressure Setpoint	0.1 to 150 psi Display the column head pressure setting in the method.
Actual Pressure	0.1 to 100 psi Display the actual column head pressure at the 450-GC.
Column Flow	Display, in mL/min, the column flow rate calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter). This value is not displayed if the column length has not been set in the 450-GC column parameters setup.
Total Flow	1 to 1000 mL/min Display the programmed total flow rate in the active method.
Linear Velocity	Display, in cm/sec, the column linear velocity calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

TCD Status

Item	Description
Ready	Yes or No.
Fault	Yes or No. Displays if a fault in the TCD detector component has occurred.
TCD Electronics	On or Off Displays the TCD Electronics setting in the active method.
Range	0.05, 0.5, or 5.0 Displays the current TCD Range setting
Time Const	Fast (50 μ sec) or Slow (200 μ sec) Displays the electrometer time constant setting from the TCD Adjustments in the active method.
Filament Temp	0 to 490 °C Displays the TCD Filament Temperature setting in the active method.
Current	Displays, in mA, the actual TCD current.
Balance Pct	Displays, in %, the TCD bridge balance. On the 450-GC, the bridge is balanced automatically each time an Autozero is performed and should normally set around 0%. A large offset in bridge balance (+ or -) could indicate a potential problem.
Polarity	Displays the current TCD Polarity setting, Positive or negative
Detector Signal	Displays, in mV, the actual TCD detector signal at the 450-GC.
Bunch Size	Displays the data acquisition bunch size.
Freq	Displays the data acquisition bunch rate, in Hz.

FID Status

Item	Description
Ready	Yes or No. The FID detector is Ready (Yes) after the setpoints are achieved and stabilized. The FID detector is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the FID detector becomes not ready or goes “out of tolerance”. Some reasons the GC may go Not Ready during a run are: the temperature program is too aggressive, the oven door is opened, the coolant runs out, the power line voltage drops, etc.
Fault	Yes or No. Displayed if a fault in the FID detector component has occurred.
FID Electronics	On or Off Display the FID Electronics setting in the active method.
Range	9, 10, 11, or 12 Display the FID Range initial condition setting or the time-programmed setting in the active method.
Time Const	Fast (50 μ sec) or Slow (200 μ sec) Display the electrometer time constant setting from the FID Adjustments in the active method.
Detector Signal	Display, in mV, the actual FID detector signal at the 450-GC.
Bunch Size	Display the data acquisition bunch size.
Freq	Display the data acquisition bunch rate, in Hz.

ECD Status

Item	Description
Ready	Yes or No.
Fault	Yes or No. Displayed if a fault in the ECD detector component has occurred.
ECD Electronics	On or Off Display the ECD Electronics setting in the active method.
Range	1 or 10 Display the current ECD Range setting.
Time Const	Fast (50 μ sec) or Slow (200 μ sec) Display the electrometer time constant setting from the ECD Adjustments in the active method.
Detector Signal	Display, in mV, the actual ECD detector signal at the 450-GC.
Bunch Size	Display the data acquisition bunch size.
Freq	Display the data acquisition bunch rate, in Hz.

TSD Status

Item	Description
Ready	Yes or No.
Fault	Yes or No. Display if a fault in the TSD detector component has occurred.
ECD Electronics	On or Off Display the ECD Electronics setting in the active method.

Item	Description
TSD Bead Power	On or Off Display the current TSD Bead Current setting
Range	9, 10, 11, or 12 Display the current TSD Range setting
Time Const	Fast (50 μ sec) or Slow (200 μ sec) Display the electrometer time constant setting from the TSD Adjustments in the active method.
Bead Current	2.4 to 3.8 A or Off Display the TSD Bead Current setting in the active method or Off if the Bead Power is off.
Detector Signal	Display, in mV, the TSD detector signal at the 450-GC.
Bunch Size	Display the data acquisition bunch size.
Freq	Display the data acquisition bunch rate, in Hz.

PFPD Status

Item	Description
Ready	Yes or No.
Fault	Yes or No. Displayed if a fault in the PFPD detector component occurred.
PFPD Electronics	On or Off Display the PFPD Electronics setting in the active method.
Range	8, 9, or 10 Display the current PFPD Range setting.
Square Root Mode	On or Off Displays the PFPD Square Root Mode setting in the active method.

Interactive Scaling

The following actions can be done in the chromatogram display window:

Action	Effect of Action
Left click and drag a selection.	Any section of the chromatogram display may be expanded to fill the chromatogram window by clicking and dragging the cursor to enclose the area of interest on the display. Whenever the display scaling is less than full scale in either axis, the appropriate scroll bar(s) will be displayed at the right or bottom of the display to allow scrolling of the display.
Left double click.	Zoom out to full scale.
Left click and hold	Zoom isometrically from the cursor, or if you are holding the control key down, zooms out from that point. After Power Zooming begins, move the cursor around while the mouse button is held down to change the zoom point.

450-GC Setup Dialog

Column Oven Zone: Temp Limit 325 C; No Coolant
 Zone 1: Front 1177: Temp Limit 350 C; No Coolant
 Zone 2: Mid 1079: Temp Limit 350 C; LN2 Coolant
 Zone 3: Rear 1041: Temp Limit 300 C; No Coolant
 Zone 4: Front FID: Temp Limit 400 C
 Zone 5: Mid FID: Temp Limit 400 C
 Zone 6: Rear ECD: Temp Limit 400 C

Front Injector EFC Type 1 Outlet: Atm, Units: psi, Splitless Vent: 10 ml/min, Gas Saver: 20 ml/min after 120.00
 Mid Injector EFC Type 1 Outlet: Atm, Units: psi, Splitless Vent: 10 ml/min, Gas Saver: 20 ml/min after 120.00
 Rear Injector EFC Type 3 is Configured with Outlet: Atm, Units: psi

Front FID Detector EFC Type 11 is Configured with Ch 1: He makeup; Ch 2: H2; Ch 3: Air
 Mid FID Detector EFC Type 11 is Configured with Ch 1: He makeup; Ch 2: H2; Ch 3: Air
 Rear ECD Detector EFC Type 13 is Configured with Ch 1: N2 makeup

Front Column is Configured with L=1500 cm, D=250 microns, H2 Carrier Gas
 Mid Column is Configured with L=1500 cm, D=250 microns, H2 Carrier Gas
 Rear Column is Configured with L=1500 cm, D=250 microns, H2 Carrier Gas

Valve 1 is Unused: Default is Off; Energized is On
 Valve 2 is Unused: Default is Off; Energized is On
 Valve 3 is Unused: Default is Off; Energized is On
 Valve 4 is Unused: Default is Off; Energized is On
 Valve 5 is Unused: Default is Off; Energized is On
 Valve 6 is Unused: Default is Off; Energized is On
 Valve 7 is Unused: Default is Off; Energized is On

Nothing connected to SID-1
 8400 Autosampler connected to SID-2 is Configured for SPME; Inj Ports in Both Positions

8400 Dual Mode Setup Print OK Rapid MS Mode Setup

The 450-GC Setup dialog displays the hardware configuration information input through the GC keyboard and currently saved in the GC memory. Use the Print button to print a copy for your records. The OK button closes the dialog. Use the other buttons to input additional configuration information.

8400 Dual Mode Setup

8400 Mounting Position:

	8400 Injection Position	Injector	Front FID Detector	Mid FID Detector	Rear ECD Detector
1	Pos 1	Front 1177	yes	no	no
2	Pos 2	Mid 1079	no	yes	no
3	N/A	Rear 1041			

Indicate which Detectors are connected to each Injector that is reachable by the 8400 Syringe Tower. This information is used to manage Data Handling for Dual-Sample Injections only (those using 'Advance' and 'Clean & Adv' modes for 2nd Injection).

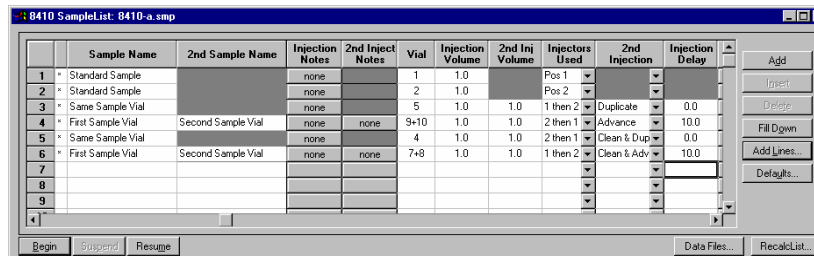
OK Cancel

The 8400 AutoSampler can inject into two contiguous injectors in the same chromatographic run. Use the 8400 Dual Mode Setup to define the configuration used when that capability is invoked. The 8400 can inject into front and middle, or middle and rear, injectors, and each of the injectors can be connected through an analytical column to any of the installed detectors.

When the 8400 AutoSampler or 8410 AutoInjector is used in Dual Mode, use this dialog box to assign the detector channels to the data file for the corresponding sample. In Dual Mode operation, two data files are created; one for the first sample injected, the other for the second sample injected. The samples that are injected are identified by their 8400/8410 Injection Position as either Position 1 or

Position 2. The user specifies which detector information to associate with each 8400/8410 Injection Position.

8400/8410 SampleList Window Extensions



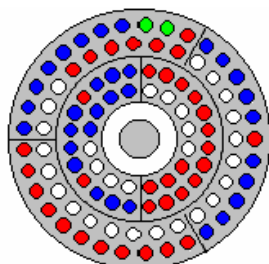
When a 450-GC controls an 8400 AutoSampler or 8410 AutoInjector, the SampleList for that instrument contains the following device-dependent fields. Many of these SampleList fields are only shown and available for editing when the 8400 AutoSampler or 8410 AutoInjector is used in Duplicate Mode or Dual Mode. See the help on the generic SampleList Window for a description of the fields that are not listed.

Field	Description
2nd Sample Name (Dual Mode operation only)	Up to 19 characters. Set the name of the second sample injected. This column is only displayed when the 2 nd Injection is "Advance" or "Clean & Adv".
2nd Inject Notes (Dual Mode operation only)	Up to 180 characters Open the Notes window for the selected second sample to edit or create a note about the sample. This column is only displayed when the 2 nd Injection is "Advance" or "Clean & Adv".
Vial	0 through 99 for 8400 AutoSampler 1 through 21 for 8410 AutoInjector Set the AutoSampler vial number of each sample in the SampleList. When the 2nd Injection is "Advance" or "Clean & Adv", two sequentially numbered vials are shown. The first vial is injected on the first injection and the next vial location is sampled for the second injection.
Injection Volume	0.1 to 5.0 μ L or 0.1 to 10 μ L or 1 to 100 μ L depending on syringe volume. Set the injection volume in microliters. When the SampleList is edited in System Control, the maximum value allowed is set to the syringe size currently configured in the 450-GC setup. If the sample volume plus solvent volume, internal standard addition volume, and air gaps volume specified in the active method on the 450-GC exceeds the syringe volume, a 450-GC hardware fault will occur. The MS Workstation halts automation and resets the 450-GC. After changing the method settings and/or the injection volume to reduce the total below the installed syringe volume shown in the 450-GC setup screen, begin the SampleList at the selected line to bypass the samples that have been run.

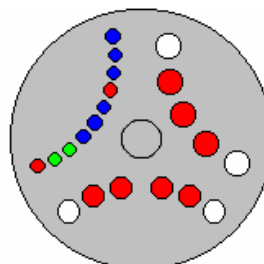
Field	Description
2nd Inj Volume (Duplicate Mode or Dual Mode operation only)	0.1 to 5.0 μL or 0.1 to 10 μL or 1 to 100 μL depending on syringe volume. Set the injection volume in microliters for the second injection of the sample in Duplicate Mode or the injection of the second sample in Dual Mode. When the SampleList is edited in System Control, the maximum value allowed is set to the syringe size currently configured in the 450-GC setup. If the sample volume plus solvent volume, internal standard addition volume, and air gaps volume specified in the active method on the 450-GC exceed the syringe volume, a 450-GC hardware fault occurs. This MS Workstation halts automation and reset the 450-GC. After changing the method settings and/or the injection volume to reduce the total below the installed syringe volume shown in the 450-GC setup screen, begin the SampleList at the selected line to bypass the samples that have been run.
Injectors Used	Pos 1, Pos 2, 1 then 2, or 2 then 1 Select the 8400 Injection position to use for the sample. If the 8400 is not configured for both injection positions, entering the wrong position skips the sample line and a "Bad Injector" message is entered into the message log. To run samples in Duplicate Mode or Dual Mode, select either "1 then 2" or "2 then 1".
2nd Injection (Duplicate Mode or Dual Mode operation only)	Duplicate, Advance, Clean & Dup, or Clean & Adv Specify what the 8400 does before making the second injection during a run. Duplicate Mode: If "Duplicate" or "Clean & Dup" is selected, the same sample is used for both injections. This is called Dual Mode: If "Advance" or "Clean & Adv" is selected, the 8400 advance to the next vial location and injects from any vial that is there for the second sample injection.
Injection Delay (Duplicate Mode or Dual Mode operation only)	0.0 and 0.1 through 10.0 minutes Set the time delay between the first injection and the second injection in Duplicate Mode and Dual Mode operation. When the value is 0.0, the injection time delay is off. For values other than zero, the 8400 prepares and loads the syringe for the second injection. When the syringe is loaded, it moves to the inject position and waits for the injection delay to time out before injecting. If the injection delay times out before the sample is injected, the error message, the injection delay timed out before injection, is put in the message log.

8400/8410 Carousel Display

When an 8400 AutoSampler or 8410 AutoInjector is connected to the 450-GC, the Carousel display is visible in the 450-GC Status and Control window.



8400 AutoSampler Carousel



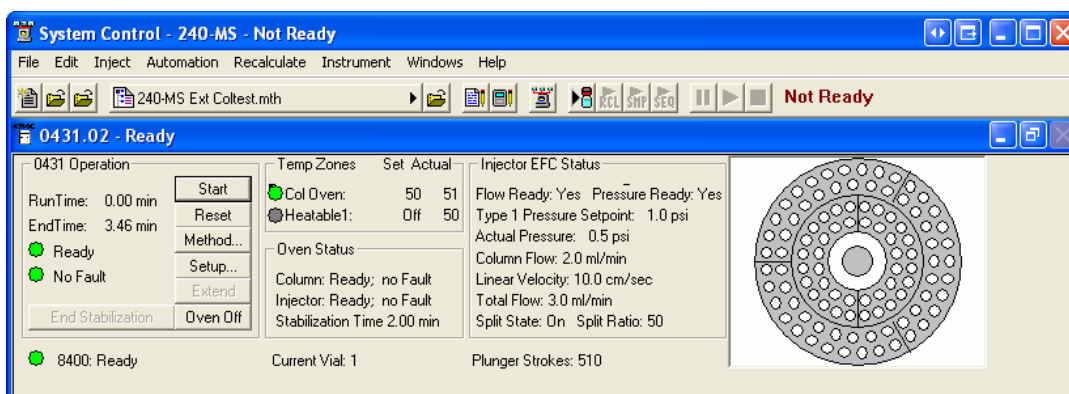
8410 AutoInjector Carousel

Item	Description
Red fill	Indicate vials, listed in the active SampleList, not sampled, or missing.
Green fill	Indicate the vial (vials in Dual Mode) being sampled.
Blue fill	Indicate the vials in the active SampleList that were sampled.

Action	Description
Click a vial position	Display the vial number for that position for 5 seconds
Double-click a vial position	Open the Inject Single Sample dialog box to inject a single sample.
Double -click center	Display the active SampleList, if selected
Double-click outside carousel	Display the active RecalcList, if selected.

431-GC System Control Command Reference

Status and Control Window



The 431-GC Status and Control window has five display areas; the 431-GC Operation display, the Temperature Zones Status display, the Injector EFC Status display, and the 8400/8410 Carousel display,

The left-most display area is the 431-GC Operation display, which has information about the current run and the overall state of the GC.

The display area to the right of the 431-GC is the Temperature Zones Status display, which has the setpoint and current actual temperature of each GC heated zone.

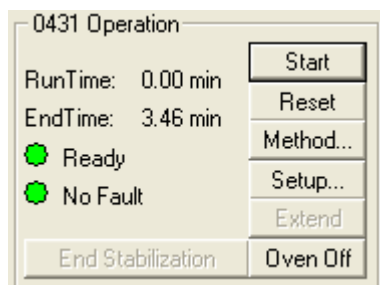
Under the temperature zone is the Oven Status.

Next is the Injector EFC Status display, which has information about the injector.

431-GCs with an 8400 AutoSampler or 8410 AutoInjector display the 8400/8410 Carousel. The display shows which vials are to be sampled, which vials have been sampled, and which vial is being sampled.

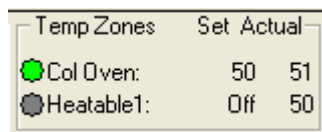
431-GC Operation Display

The 431-GC Operation display is in the left portion of the 431-GC Status and Control window.



Item	Description
Run Time	The elapsed time in minutes after the run started. The maximum run time is 999.99 minutes.
End Time	The time the run ends.
State	Ready, Running, Stabilizing, Equilibrating, Computing, Needs Monitor, Monitoring, Sampling, Connecting, or Not Ready The state of the GC. The light is green if the GC is Ready or Running. Otherwise, the light is red.
Fault/No Fault indicator	No Fault (green light) or Fault (red light). When a hazardous or disabling fault occurs, any run in progress is halted and the affected component shut down. If the fault is recoverable, then the run is not terminated.
Start	If the system is Ready, starts the GC Method and sends a start signal to the GC. Equivalent to pressing Start on the front panel of the GC. The Start button is disabled unless the GC is in the Ready state.
Reset	Reset the GC, advancing it to the next state. If RUNNING, the GC aborts the current run, goes to the READY state, and continues with the next injection in the Sequence. Equivalent to pressing Stop on the front panel of the GC.
Method	Open the Method Builder application to edit the active method.

Temperature Zones Status Display



Temperature zones includes the setpoints and actual temperatures of the column oven, the three zones that can be cooled or heated, and the three zones that only be heated. The display is **Fault** if a fault occurs, or **Off** if the zone oven is off. If the zone was not configured by the 431-GC, then **N/A** is displayed for the setpoints and actual temperature. Click a temperature zone entry to display the corresponding component status in the Component Status Display.

The LEDs indicate the status of each temperature zone. If the zone is not configured or the zone oven is off, the LED is gray. If the temperature zone is Not Ready or there is a fault, the LED is red. Otherwise, the LED is green.

Injector EFC Status Display

Injector EFC Status	
Flow Ready: Yes	Pressure Ready: Yes
Type 1 Pressure Setpoint: 1.0 psi	
Actual Pressure: 0.5 psi	
Column Flow: 2.0 ml/min	
Linear Velocity: 10.0 cm/sec	
Total Flow: 3.0 ml/min	
Split State: On	Split Ratio: 50

Item	Description
Ready	Yes or No. The Type 21 or 25 EFC Injector is Ready (Yes) if the setpoints were achieved, and stabilized.
Fault	Yes or No. Displayed if a fault in the Type 21 EFC component has occurred.
Type 1 Pressure Setpoint	0.1 to 100 psi Display the programmed column head pressure setting in the active method.
Actual Pressure	0.1 to 100 psi Display the actual column head pressure in the GC.
Column Flow	Display, in mL/min, the column flow rate calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).
Linear Velocity	Display, in cm/sec, the column linear velocity calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).
Total Flow	Display, in mL/min, the total flow rate through the system.
Split State	On or Off. Display the current split state of the 1177 injector method.
Split Ratio	1 to 10000 Display the current split ratio of the 1177 injector method. The split ratio is defined as the (Column Flow + the Split Flow) / the Column Flow.

AutoSampler Status

● 8400: Ready
 Current Vial: 1
Plunger Strokes: 510

This option is only shown on 431-GCs that have an 8400 AutoSampler or 8410 AutoInjector connected to them.

Item	Description
8400/8410 State	Ready or Running
Current Vial	0 through 99 for 8400 AutoSampler 1 through 21 for 8410 AutoInjector
Plunger Strokes	Displays the number of times that the syringe plunger has been stroked up and down. This can be used to help monitor syringe wear and plan for syringe replacements.
Tray Orientation (8410 AutoInjector Only)	Vials 1 through 10, Vials 11 through 16, or Vials 17 through 21 Shows the range of vials accessible from the current 8410 carousel location.

8400 Dual Mode Setup

8400 Dual Mode Setup
✕

8400 Mounting Position: Front

	8400 Injection Position	Injector	Front FID Detector	Mid FID Detector	Rear ECD Detector
1	Pos 1	Front 1177	yes	no	no
2	Pos 2	Mid 1079	no	yes	no
3	N/A	Rear 1041			

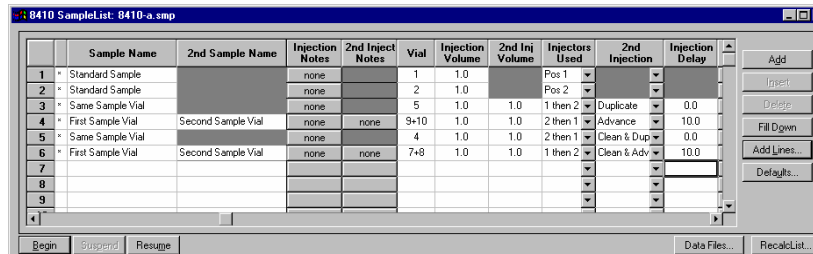
Indicate which Detectors are connected to each Injector that is reachable by the 8400 Syringe Tower. This information is used to manage Data Handling for Dual-Sample Injections only (those using 'Advance' and 'Clean & Adv' modes for 2nd Injection).

OK
Cancel

The 8400 AutoSampler can inject into two contiguous injectors in the same chromatographic run. The 8400 Dual Mode Setup dialog allows you to define the configuration to be used when that capability is invoked. The 8400 can inject into front and middle, or middle and rear, injectors, and each of the injectors can be connected through an analytical column to any of the installed detectors.

When the 8400 AutoSampler or 8410 AutoInjector is used in Dual Mode, use this dialog box to assign the detector channels to the data file for the corresponding sample. In Dual Mode operation, two data files are created; one for the first sample injected, the other for the second sample injected. The samples that are injected are identified by their 8400/8410 Injection Position as either Position 1 or Position 2. The user specifies in the table which detector information to associate with each 8400/8410 Injection Position.

8400/8410 SampleList Window Extensions



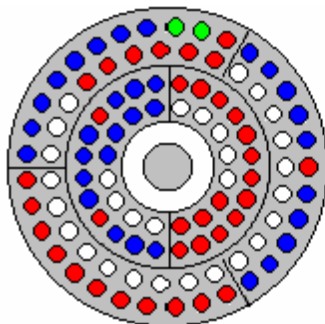
When a 450-GC controls an 8400 AutoSampler or 8410 AutoInjector, the SampleList for that instrument contains the following device-dependent fields. Many of these SampleList fields are only shown and available for editing when the 8400 AutoSampler or 8410 AutoInjector is used in Duplicate Mode or Dual Mode. See help on the generic SampleList Window for a description of the fields not listed.

Field	Description
2nd Sample Name (Dual Mode operation only)	Up to 19 characters Set the name of the second sample injected. This column is only displayed when the 2 nd Injection is "Advance" or "Clean & Adv".
2nd Inject Notes (Dual Mode operation only)	Up to 180 characters Open the Notes window for the selected second sample to edit or create a note about the sample. This column is only displayed when the 2 nd Injection is "Advance" or "Clean & Adv".
Vial	0 through 99 for 8400 AutoSampler 1 through 21 for 8410 AutoInjector Set the AutoSampler vial number of each sample in the SampleList. When the 2nd Injection is "Advance" or "Clean & Adv", two sequentially numbered vials are shown. The first vial is injected on the first injection and the next vial location is sampled for the second injection.
Injection Volume	0.1 to 5.0 μ L or 0.1 to 10 μ L or 1 to 100 μ L depending on syringe volume Set the injection volume of the sample in microliters. When the SampleList is edited in System Control, the maximum value allowed is set to the syringe size currently configured in the 450-GC setup. During operation, if the sample volume plus solvent volume, internal standard addition volume, and air gaps volume specified in the active method on the 450-GC exceeds the syringe volume, a 450-GC hardware fault will occur. This will cause the Star Workstation to halt automation and reset the 450-GC. After changing the method settings and/or the injection volume to reduce the total below the installed syringe volume shown in the 450-GC setup screen, you should begin the SampleList at the selected line to bypass the samples that have already been run.

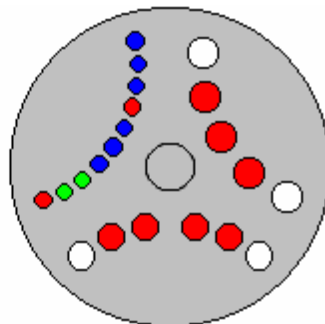
2nd Inj Volume (Duplicate Mode or Dual Mode operation only)	0.1 to 5.0 μL or 0.1 to 10 μL or 1 to 100 μL depending on syringe volume Set the injection volume in microliters for the second injection of the sample in Duplicate Mode or the injection of the second sample in Dual Mode. When the SampleList is edited in System Control, the maximum value allowed is set to the syringe size currently configured in the 450-GC setup. During operation, if the sample volume plus solvent volume, internal standard addition volume, and air gaps volume specified in the active method on the 450-GC exceed the syringe volume, a 450-GC hardware fault occurs. This causes MS Workstation to halt automation and reset the 450-GC. After changing the method settings and/or the injection volume to reduce the total below the installed syringe volume shown in the 450-GC setup screen, begin the SampleList at the selected line to bypass the samples that have been acquired.
Injectors Used	Pos 1, Pos 2, 1 then 2, or 2 then 1 Select the 8400 Injection position used for the sample. If the 8400 is not configured for both injection positions, entering the wrong position causes the sample line to be skipped and a "Bad Injector" message to be entered into the message log. To run samples in Duplicate Mode or Dual Mode, select either "1 then 2" or "2 then 1".
2nd Injection (Duplicate Mode or Dual Mode operation only)	Duplicate, Advance, Clean & Dup, or Clean & Adv Specifies the action that the 8400 takes before making the second injection during a run. Duplicate Mode: If you choose "Duplicate" or "Clean & Dup", the same sample is used for both injections. Dual Mode: If you choose "Advance" or "Clean & Adv", the 8400 advances to the next vial location and samples from that vial, if any, that is there for the second sample injection.
Injection Delay (Duplicate Mode or Dual Mode operation only)	0.0 and 0.1 through 10.0 minutes Set the time delay between the first injection and the second injection in Duplicate Mode and Dual Mode operation. When the value is 0.0, the injection time delay is turned off and not used. For values other than zero, the 8400 prepares and loads the syringe for the second injection. After the syringe is loaded, it moves to the inject position and waits for the injection delay to time out before injecting. If the injection delay times out before the sample is injected, an error message saying that the injection delay timed out before injection is put in the message log.

8400/8410 Carousel Display

When an 8400 AutoSampler or 8410 AutoInjector is connected to the 450-GC, the Carousel display is shown in the 450-GC Status and Control window.



8400 AutoSampler Carousel



8410 AutoInjector Carousel

Item	Description
Red fill	Indicate vials, listed in the active SampleList, not sampled, or missing.
Green fill	Indicate the vial (vials in Dual Mode) currently being sampled.
Blue fill	Indicate the vials in the active SampleList that were sampled.

Action	Description
Click a vial position	Display the vial number for that position for 5 seconds
Double-click a vial position	Open the Inject Single Sample dialog box to inject a single sample.
Double -click in center	Display the active SampleList, if one is selected
Double-click outside carousel	Display the active RecalcList, if one is selected.

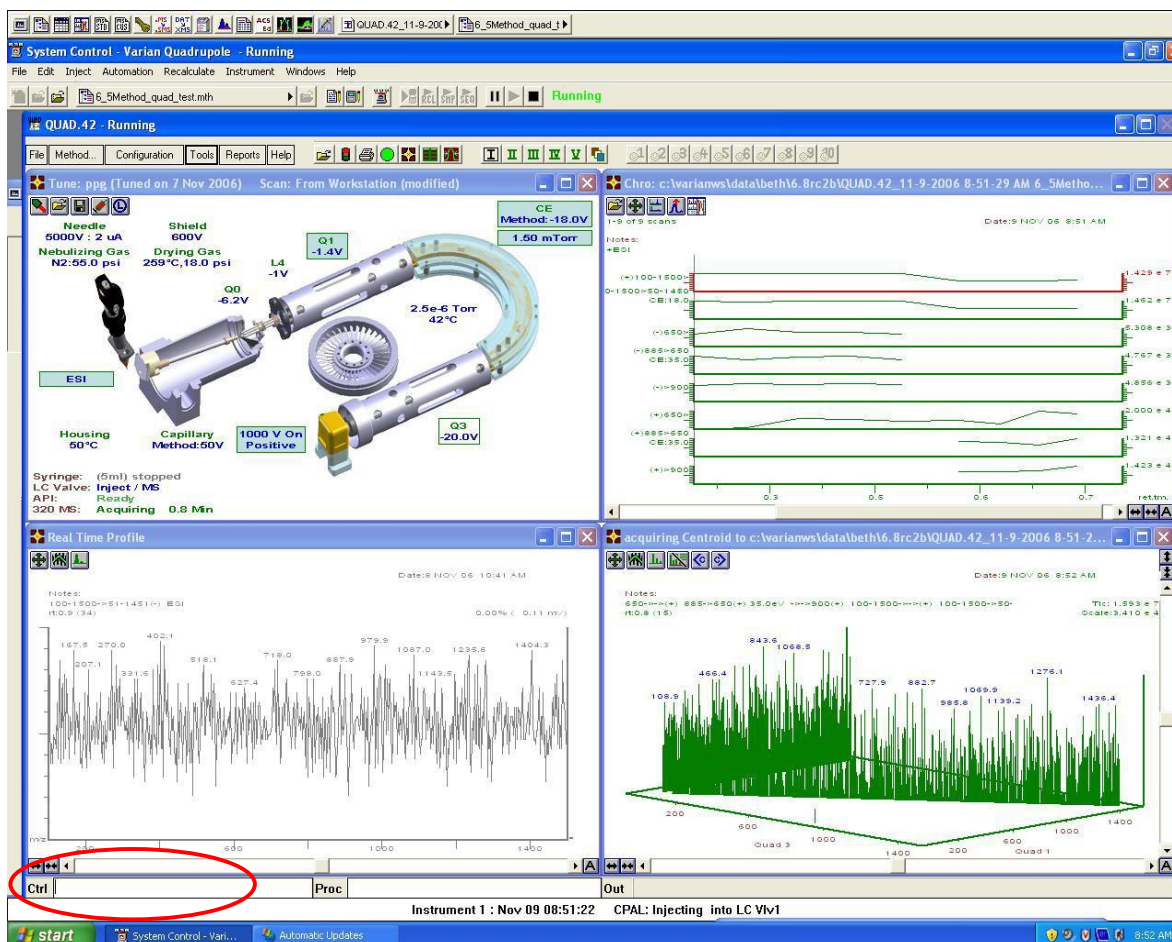
PML

Overview of PML

The procedures that generate information reporting results from the mass spectrometer are written in a language called Paw Macro Language (PML). It has commands that control the instrument or data processing. Users can write procedures to customize data processing.

Simple Commands

Simple commands can be entered in the **Ctrl** field.



Typing "Hello" (quotes included) in the **CTRL** text box prints Hello in the **Out Status** display on the task bar.

CANCEL stops the Paw macro running at the top level.

QUIT stops all paw macros. If you use the *Quit* key word, type *scan* to restart the system.

PML Syntax

The macros are text files with the extension.pml. There are macros in the PML Directory (default: C:\VarianWS\1200sys\PML). If you create your own macros or make new versions of the existing ones, store them in the User PML Directory (default: C:\VarianWS\UserPML). Macros can be edited using the **Pml Editor** described later in this section.

The names can contain letters, numbers, or underlines, but they must begin with a letter.

Run a macro by typing the name of the command lines of the instrument window (CTRL) or including the name in another macro. You can send arguments to a macro and it will return a value.

Paw Macros Consist of Statements:	Examples:
Action or function keywords:	OFF DOZE(2.5)
Macro calls:	CGON SW(219)
Assignment statements:	DETECTOR = 1000 DETECTOR += 50 DETECTOR -= 50 x = COS(PI)
Conditional Statements:	IF (WIDTH > 10) ELSE WHILE (x < 100 & y <= 100) UNTIL (x = 100 y != 100) REPEAT 100 REPEAT
Completing Statements:	END terminates a conditional statement
	RETURN(n) returns from a subroutine with result n
	CANCEL stops the paw macro running "at the top level"
	QUIT stops all paw macros
Printing statements:	?DETECTOR prints the current detector value on the display.
	"Hello" prints Hello on the display.

The Statements Refer To:

numerical values	e.g.	20, -3.5, 1000H
variable keywords	e.g.	DETECTOR
function keywords	e.g.	COS
action keywords	e.g.	FISH
macros	e.g.	STANDBY
user variables	e.g.	X,Y
arguments	e.g.	%1,%2,%3,%4,%5

Notes

1. Statements are separated from each other by colons, semicolons, or line breaks.
2. Conditional statements must have a matching END statement:
 - if (x < y) & ~(x = 2) : fish : else : scanlens : end
 - if x = 3 : sw(502) : end
 - i = 1 : repeat 100 : sn = i: list(i) = tic : i += 1 : end

END statements at the bottom of a PAW Macro can be deleted.

3. Printing statements (using ? and "") can be strung together. They are terminated with the keyword CR (carriage return).
4. Some keywords create text like the printing statements using ? and ".".

GET_FILENAME
LIB_FORMULA
LIB_NAME
LIST_TO_STRING
SAMPLE_NAME
STRING_RESTORE
SUB_FILE_NAME
VERSION

5. Some keywords re-route the text created by printing statements (using ? and ") to other places than the display.

DACS_RESTORE : "file name" : CR
DACS_SAVE : "file name" : CR
FILE_APPEND : "file name" : CR
FILENAME : "file name" : CR
FILE_OPEN : "file name" : CR
IONS_RESTORE : "file name" : CR
IONS_SAVE : "file name" : CR
LCD : "message" : CR
LIB_FIND : "compound name" : CR

LIST_RESTORE	: "file name" : CR
LIST_SAVE	: "file name" : CR
MSGBOX	: "label text" : CR : "default": CR:
"Macro":	CR
PICT_LABEL	: "label text" : CR
PICT_TITLE	: "title text" : CR
STRING_SAVE	: "text" : CR (ten user strings)
STRING_TO_LIST	: "text" : CR
SUB_NAME	: "text" : CR

6. Statements may include comments. A # ends the statement and starts the comment, e.g., :DETECTOR += 10 # raise the detector to make the peak bigger.
7. All numerical values referred to in PAW Macros are real numbers. Usual algebraic syntax is allowed:, e.g., $x = (\sin(y) + \cos(\sqrt{\text{detector}})) / (30 * \text{month} + \text{day})$.
8. When parameters are passed to macros, they are referred to within the macro as %1, %2, %3, %4 and %5. e.g., if the macro TIMES is defined as ?%1 : "times" : ?%2 : "equals" : ?(%1 * %2) : CR and you type "TIMES 7 9" and the instrument will print out "7 times 9 equals 63". NOTE: %1 - %5 can be used as local variables within any macro.
9. When passing parameters to a macro or keyword, you can leave out parentheses at the top level.

All these are valid statements:

```
FISH(3)
FISH 3
FISH 3 2
FISH 3,2
FISH(3,2)
```

When assigning a value to a variable or parameter you can leave out the = sign.

```
DETECTOR = 1000
DETECTOR 1000
```

but: "lens(1) = 100" is ok while "lens 1 100" is ambiguous.

10. When using printing statements on the control line, or if the string you type starts with? or " or VERSION, you don't have to type the terminating CR.

System Paw Macros

1. When the Status Window is opened, a Ctrl: PML (default: INIT) and a Proc: PML (default: QUAN_INIT) are both run.
2. In the Collect menu (toolbar start button) a Ctrl: PML is defined which runs when the file being collected is opened.
3. In the queue menu (Collect Queue edit button) a Proc: PML is defined which runs when the file being collected is closed.
4. A Windows application outside the instrument can request a PML through the windows DDE mechanism.
5. Using the MSGBOX keyword you create and run PMLs.
6. Some PMLs run when you click on buttons or menu items:

File menu Reset: INIT

File menu Standby: STANDBY

Status control menu: CGON CGOFF CION CIOFF CIDON CIDOFF

AutoTune menu: ATUNE1 ATUNE2 ATUNE3 ATUNE4 ATUNE5 ATUNE6

Diagnostic menu: DIAGNOSTIC(test_number)

Tune Table menu optimize button: OPTIMIZE

Status probe button: PROBE_MAIN

Species Boiling Pt. Range menu compute button: SHELL

Clicking in Chro: CHRO_CLICK(sn,rt,type_rt + (10*type_sn) + (1000*make_substance))

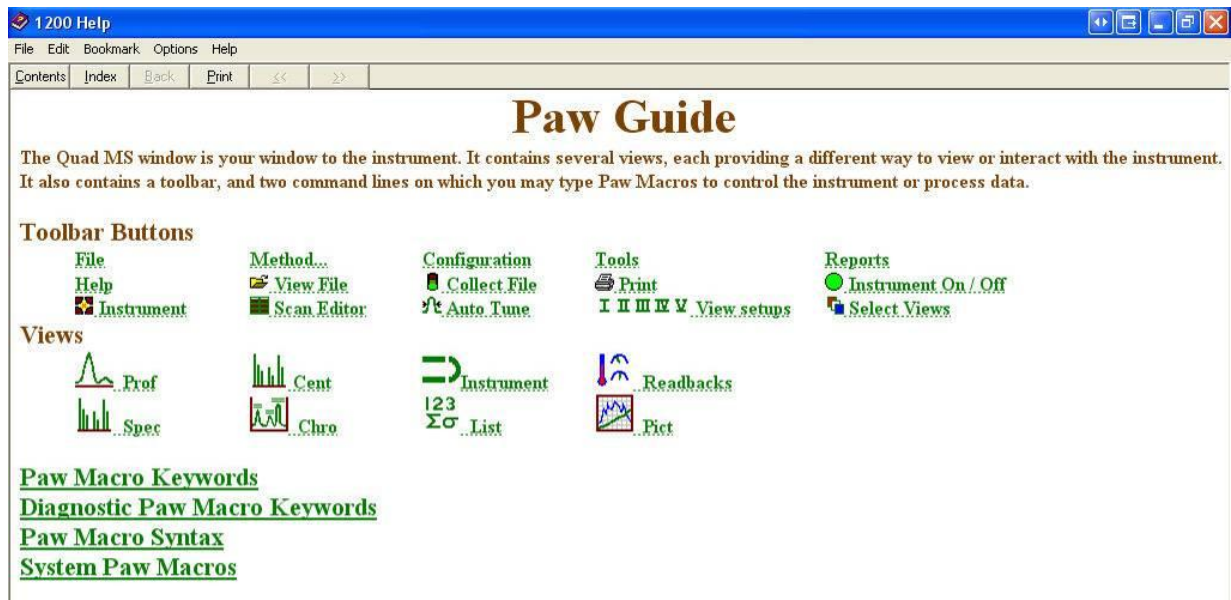
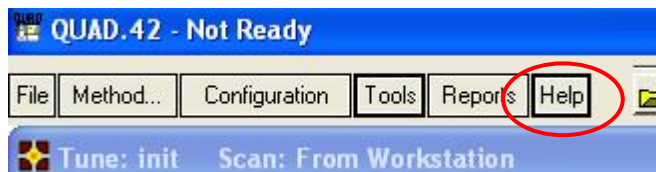
(click on the CHRO scales button to see where type_rt,type_sn, and make_substance are defined)

Other popular PMLs are:

BL	PAR
DAU	QIMS
FM	Q3MS
LM	SCAN
MIXED	SW
NL	

Help Files for PML

Click **Help** in the System Control window to open the Paw Guide.



Some PML Procedures

The Cioff.pml macro closes the CI gas valve, prints "Evacuating CI Gas (takes 5 seconds)" in the status area of the taskbar, opens and closes the vent valve, and prints "CI gas off" in the status area of the taskbar.

CIOFF.pml

valve 2 = 0	# close CI valve
"Evacuating CI Gas (takes 5 seconds)";cr	#printing statement, terminated with the keyword CR (carriage return)
doze 1	#wait one second
valve 4 = 1	# open CI vent valve for 0.2 seconds
doze .2	
valve 4 = 0	# close vent valve for one second
doze 1	
valve 4 = 1	# open vent for 3 seconds
doze 3	
valve 4 = 0	# finally close vent
"CI Gas off!";cr	#printing statement, terminated with the keyword CR (carriage return)

The LEAK.pml assists in finding vacuum system leaks. It sets a series of masses from a compound or mixture used for leak detection. First, the Pict view window is cleared, the title in the Pict window is set, centroid mode is set, mass range is set, the parameters are optimized to prevent saturation, and a series of mass intensities are plotted while the user sprays a gas at possible leak locations.

LEAK.pml

pict_clear	# clear the picture/graph window
pict_title:"1->mass 18, 2->mass 28, 3->mass 33, 4->mass 45, 5->tic";cr	#Sets the title in the pict view
cent	#Go to centroid mode
fm 10	#Set first mass (FM) to 10
lm 50	#Set last mass (LM) to 50
optdet	#Optdet runs opt_detector.pml to prevent detector saturation after each scan.
repeat	#repeat items below
fish	#go get one scan of data
pict(,area(18),1)	#get area of mass 18 and plot point in pict view position 1
pict(,area(28),2)	#get area of mass 28 and plot point in pict view position 2
pict(,area(33),3)	#get area of mass 33 and plot point in pict view position 3
pict(,area(45),4)	#get area of mass 45 and plot point in pict view position 4
pict(,tic,5)	#get area of mass total ion current (tic) and plot point in pict view position 5
end	

Mixed.pml gets one scan in centroid data and one scan of profile data.

MIXED.pml. When Prof and Cent views are selected in the window, both real time centroid and Profile data is observed.

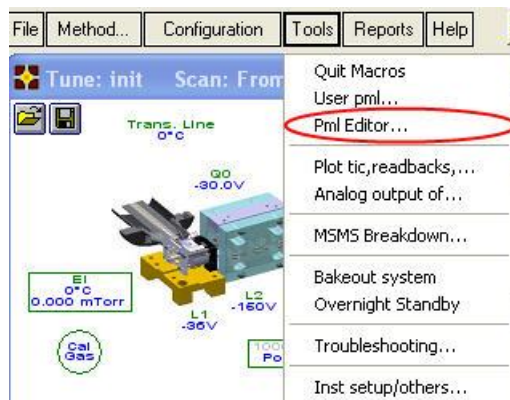
Repeat	#repeat items below
Prof	#set to scan of profile data
Fish	#go get one scan of data
Cent	#set to scan of centroid data
Fish	#go get one scan of data
End	

PML Editor

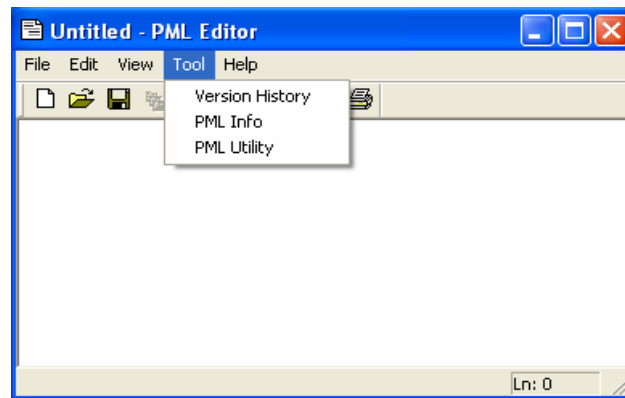
The **PML Editor** is used for creating and editing PMLs for the 300 Series software. The PML Editor allows access to the factory PML files; however, if a factory PML is modified it will then be saved as a user PML in the UserPML directory.

Accessing the PML Editor

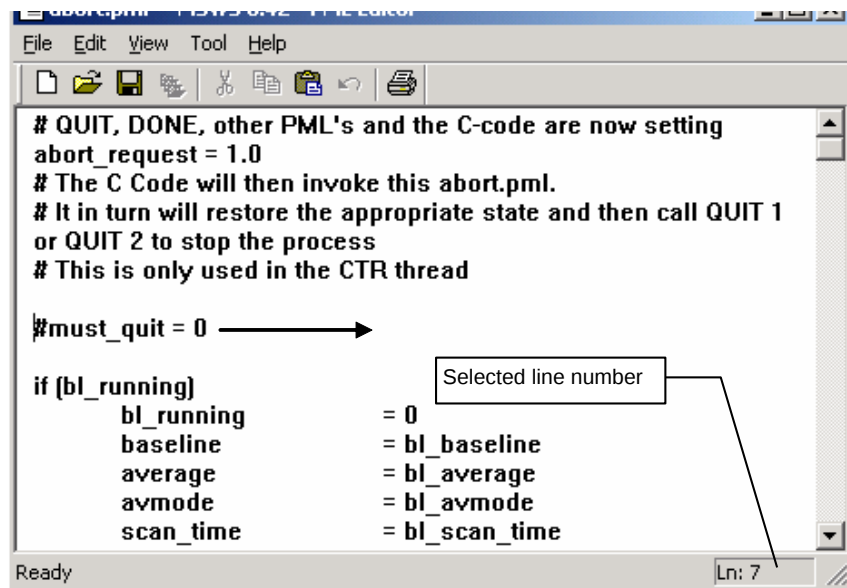
Click **Tools** in the Quad module window to display the PML editor.



The PML editor window opens.

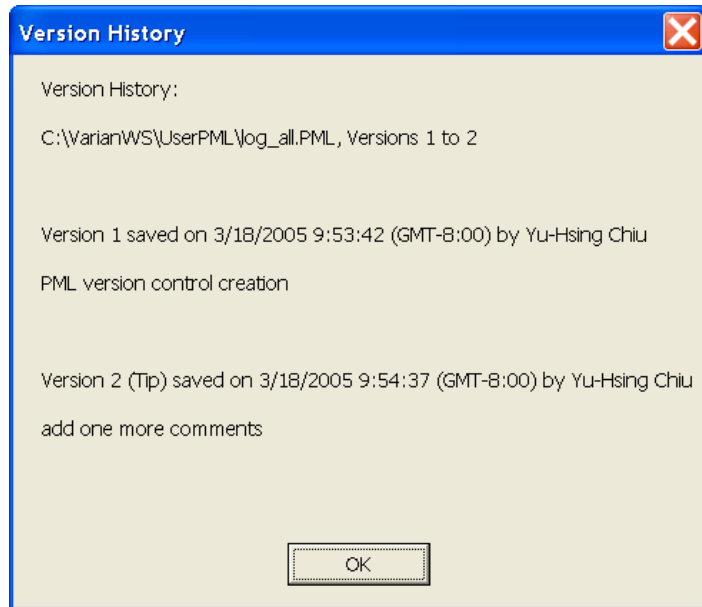


- Varian PMLs are stored in c:\varianws\1200sys\PML directory.
- User created PMLs or modified factory PMLs are stored in c:\varianws\UserPML directory.
- The Status Bar of the PML Editor displays the line number of the current cursor position.

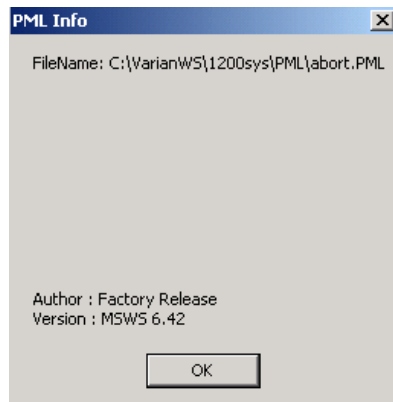


- The Tool menu has three menu items:

Version History: If the 21CFR11 application is enabled, click this to display the version history of the currently open PML.



PML Info: Display the PML path name, release version number, and any descriptions that have been in the PML header section. (Lines begin with ##).



PML Utility: Use this to perform syntax checking of the currently open PML and produce a call tree, PML keywords and User Variables defined in the PMLs. For the keywords listed, user can select and use F1 to get online help about the keywords.

In the right part of the utility dialog box, user can enter a specified keyword, and find out the PMLs contain this keyword.

