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Agilent Technologies

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210-MS, 220-MS, and 225-MS GC/MS Ion Trap Mass Spectrometer

MS Workstation

Version 6

Software Operation Manual

QUALITY SYSTEM
ISO 9001
CERTIFIED

Printed in U.S.A. 03-954145-00:3

Trademark Acknowledgments

Contents

Getting Started

About this Manual/Help

This manual/help system contains information about acquiring data, building methods, and operating the 210-MS, 220-MS, and 225-MS with the Varian MS Workstation. This manual also describes the configuration of the 450-GC and 431-GCs for standard Ethernet communication with the MS and MS Workstation's System Control application.

Use this manual with the other manuals supplied with MS Workstation and the 450-GC or 431-GC. This information in this manual is also available in the On-Line Help section of the software.

Additional Manuals/Help

Other sources of information include the following:

210-MS, 220-MS, and 225-MS Ion Trap Mass Spectrometer Hardware Operation Manual/Help

The manual/Help system provides the necessary information for installing, maintaining, using, and repairing your MS hardware. All of the information included in this manual is also available in the On-Line Help section of the software.

MS Workstation Software Reference

This reference manual provides information about data handlng in MS Workstation. It includes specific information about examing data files with MS Data Review, library searches, quantitation, and TurboDDS™.

MS Workstation Tutorial Manual

This manual/Help system provides a practical way to quickly learn how to perform basic tasks using the MS Workstation Software. While these tutorials use Saturn 2000 ion trap files, they can easily be adapted to your instrument configuration.

450-GC and 430-GC User Manuals

These manuals are included on the Varian MS Workstation CD-ROM and describe the GC Method, instrument operation, and the process of connecting your GC to a PC or to an existing network.

Context Sensitive Help

The MS Data Review, Method Builder and System Control sections of the software contain Context Sensitive Help. Help can be obtained simply by positioning the mouse pointer on the item of interest, clicking the right mouse button and selecting "What's This."

Configuring the GC/MS

Starting System Control the First Time

Before opening System Control for the first time, confirm the instrument configuration. Ensure that any instrument modules that are not part of the system have been disabled. To enable or disable instrument modules refer to the Workstation Toolbar section, “Using MS Workstation Toolbar” on page 23. In this section, GC refers to either the 450-GC or the 431-GC.

Configuring the Instrument

Before configuring the system, determine if you are going to put the Workstation on a company network or an isolated network. Use this table to determine the order in which you should read the following sections.

1. If an Ethernet card has not been installed and configured on your PC, read “Installing and Configuring the Ethernet Card in Your PC” on page 11 and the correct option:
   - ” Configuring TCP/IP Parameters with no Company Network” on page 12.
   - “Configuring TCP/IP Parameters for a Company Network” on page 14.
2. Read “Connecting Your GC to Your PC or Network” on page 14.
3. If you have not already installed the Varian MS Workstation, do so before proceeding.
   - No Company Network: See ” Configuring the GC Communication (No Company Network)” on page 14.
   - Company Network: See “Configuring the GC for a Company Network” on page 16.
4. Continue reading the rest of the sections, starting with “Adding a GC and MS in System Control” on page 20.

Installing and Configuring the Ethernet Card

NOTE: This is a generic description. Refer to the Windows and Ethernet card documents for more detailed information.

Refer to the installation instructions packaged with your Ethernet card for information on installing the Ethernet card in your computer. Before proceeding,

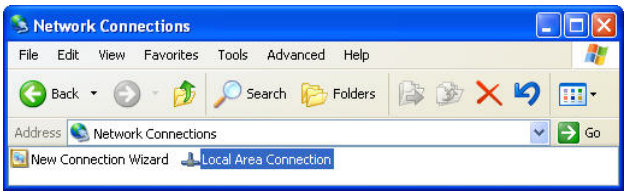
your Ethernet card should be recognized by your Windows version. When done, the **Network Neighborhood** icon should appear on your Windows desktop.

NOTE: For the following procedure, using disks other than the ones that were used for the original Windows installation may result in an Ethernet driver version mismatch that prevents Windows from starting. Should this occur, it may be necessary to remove the Ethernet Board from the computer to remove the incorrect Ethernet drivers.

To configure the network settings for communication with the GC:

1. Click **Control Panel** from the **Start** menu.
2. Double-click **Network Connections**.

3. Double-click **Local Area Connection**.



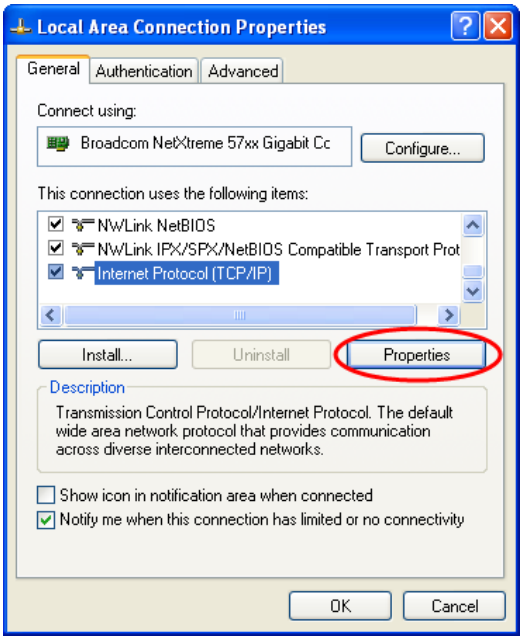
4. Click **Properties** under the **General** tab.
5. If Internet Protocol (TCP/IP) is not displayed in the list of items, click **Install** and then continue to the next step. If Internet Protocol (TCP/IP) is displayed, you are finished.
6. Select **Protocol**, and then click **Add**.
7. Click **Have Disk** if you have an installation disk for this component or click the Protocol you want to install and click **OK**.

NOTE: If not connecting Workstation to a company network (that is, you are not assigned an IP address by a Network Administrator), continue to the next section. If connecting Workstation to a company network, go to “Configuring the GC for a Company Network” on page 16.

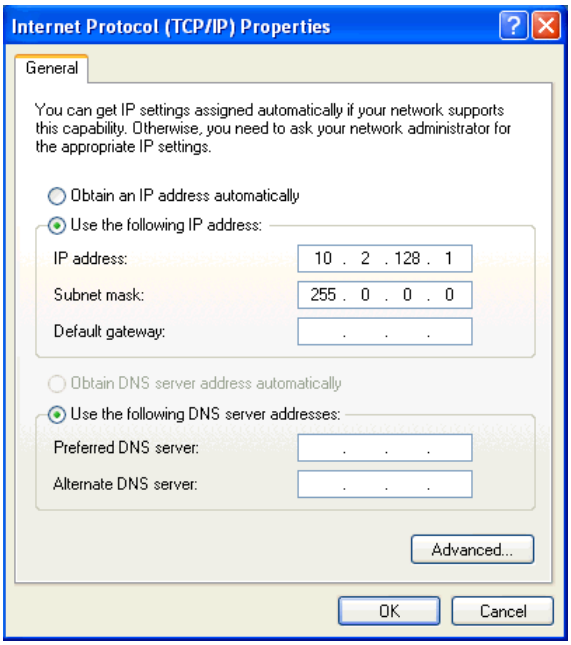
Configuring TCP/IP Parameters with no Company Network

After completing steps 1 through 5 for Installing and Configuring the Ethernet Card in Your PC continue as follows:

1. Select **TCP/IP** from the network components list and click **Properties**.



2. Enter an IP address in the range **10.2.128.1** through **10.255.255.254**. If adding more than one Workstation to this network, **each Workstation PC must have a unique IP address within this range.** The Subnet Mask is automatically set to 255.0.0.0. **Do not change this value.**



3. Ensure that there are no entries in the Gateway, and that Domain Name Server (DNS) and WINS Configuration are disabled.

NOTE: These entries are not used in an isolated network. They may cause problems if they are present.

4. Delete settings from a previous configuration.
5. Click **OK** in the Network dialog box.
6. Reboot Windows for the changes to take affect.

NOTE: Refer to *Communication Problems* in the *Diagnostic and Troubleshooting* section for information about diagnostic tools to verify that your network installation is correct.

Configuring TCP/IP Parameters for a Company Network

After completing steps 1 through 6 for Installing and Configuring the Ethernet Card in Your PC continue as follows:

1. Select TCP/IP from the network components list and click Properties.
2. Contact your Network Administrator (or whoever assigns IP addresses in your network) to get the appropriate address. **Note that each Workstation PC must have a unique IP address.** Enter the appropriate Subnet Mask to be used with this IP address.
3. Obtaining an IP address.
    - Your Network Administrator may instruct you to obtain an IP address automatically by clicking **Obtain an IP address automatically**.

NOTE: Contact your Network Administrator (or whoever assigns IP addresses for your network) to see what the appropriate settings are for your Gateway, and whether Domain Name Server (DNS) and WINS Configuration are needed.

    - Your Network Administrator may instruct you to specify parameters in the **Advanced** window.
4. Reboot Windows for the changes to take affect.

NOTE: Refer to *Communication Problems* in the *Diagnostic and Troubleshooting* section for information about diagnostic tools to verify that your network installation is correct.

Connecting the GC to the PC or Network

Refer to the “Communications” section of the *Operator’s Manual* of your GC for instructions on connecting your GC to the PC or a company network. Before proceeding, your GC should be connected to your PC or network.

Configuring the GC Communication (No Company Network)

Use the following instructions if both the GC and Varian MS Workstation PC are not on a company network dedicated to Varian MS Workstations and the instruments they control. In this case, a Network Administrator does not assign IP addresses.

NOTE: If connecting your GC and Varian MS Workstation PC to a multi-purpose company network managed by a Network Administrator, refer to Configuring the GC Communication for a Company Network.

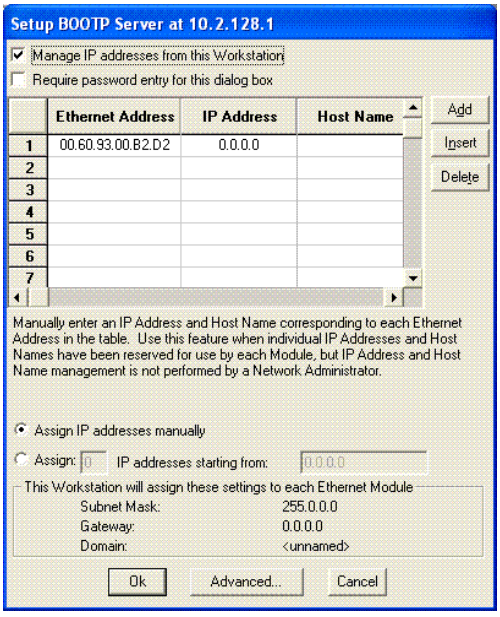
One GC can be directly to one Workstation.

1. After configuring your computer's network settings, click **System Control**.

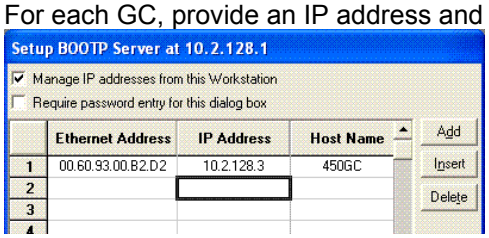
2. When opening **System Control** for the first time, use the Configuring Communication Wizard to guide you through the setup and network connections of your GC.
3. Click **Next** until the **Setup Ethernet Ports** window opens.
4. Click **Setup.**
5. Click **Manage IP addresses from this Workstation** check to manage the IP address from this workstation.

NOTE: If more than one Workstation is being connected on the same network, only one Workstation should manage the IP addresses for all connected GCs (others should have the *Manage IP addresses from this Workstation* checkbox **unchecked**). If more than one Workstation is managing IP addresses, naming conflicts may arise.

6. When the GC is powered on, an entry is added to the table.



7. For each GC, provide an IP address and a host name to identify it.



8. Click **OK**. The GC is now configured for communications and can now be selected from the **Setup Ethernet Ports** dialog box.

NOTE: Proceed to "Using a Password to Protect BOOTP Settings" on page 19.

Configuring the GC for a Company Network

Do the following to connect both the GC and MS Workstation PC are to a *company network*, that is, a multi-purpose network used for services in addition to instrument control. In this case, a Network Administrator assigns IP addresses. If the GC and the MS Workstation computer are the only devices being connected, refer to "*Configuring the GC Communication (No Company Network)"* on page 14.

You may connect virtually any number of 450-GCs or 431-GCs and any number of Varian MS Workstation computers to a company Ethernet network.

Depending on the network configuration, all MS Workstations may control all 450-GCs or 431-GCs on the network.

1. After configuring the network settings, click **System Control**.

2. If opening System Control for the first time, use the Wizard to guide you through the setup and network connections of your GC.

NOTE: Before proceeding with this section, consult your Network Administrator about whether a central BOOTP Server is available on the network.

3. If IP addresses are managed by a central BOOTP Server, then proceed to *Specifying IP Addresses from a Central BOOTP Server*.
4. If IP addresses are specified by a Network Administrator but not centrally managed, then continue reading *Specifying IP Addresses from System Control*.

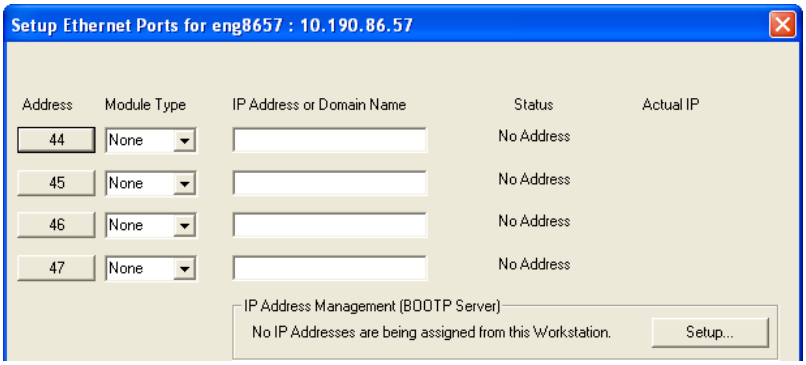
Specifying IP Addresses from System Control

Use MS Workstation to specify the IP addresses for the 450-GCs and 431-GCs attached to the network.

Use the following procedure to manage IP addresses from System Control.

1. When System Control opens for the first time, use the Configuring Communications Wizard to guide you.

2. Click **Next** until the **Setup Ethernet Ports** window opens.
3. Click **Setup** to display the **BOOTP Server** dialog box.



4. Check **Manage IP addresses from this Workstation** box to enable the BOOTP Server. The BOOTP Server has a table listing all GCs to which IP addresses may be assigned. If GCs are already connected to the network and powered on, their Ethernet addresses will appear in the table.

NOTE: If more than one Workstation is being connected on the same network, only one Workstation should manage the IP addresses for all GCs connected (all others should have the *Manage IP addresses from this Workstation* checkbox **unchecked**). The Workstation acting as BOOTP Server must run all the time to allow other Workstations to connect to GCs. If more than one Workstation is managing IP addresses, naming conflicts may arise.

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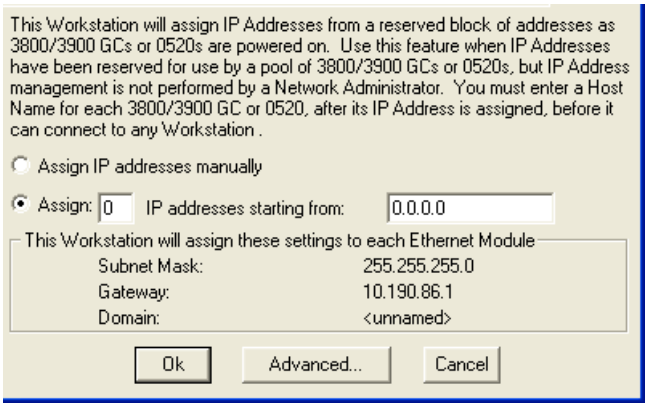
5. Enter a host name for each GC. IP addresses are not assigned to a GC until a name is entered. manually enter the ethernet address of any GC, or it can be automatically entered when a GC is powered on and broadcasts its ethernet address. Manually assign any IP address to any GC.
6. Click **OK** after entering all addresses and names.
7. If you select **Assign IP addresses starting from** the bottom portion of the dialog changes.

8. Enter the number of IP addresses you want to automatically assign. Enter the starting address here. As the GCs are powered on, IP addresses are assigned consecutively starting with this address.



NOTE: Proceed to “Using a Password to Protect BOOTP Settings” on page 19.

Specifying IP Addresses from a Central BOOTP Server

If IP addresses are managed by a Network Administrator from a central source, the GCs must be added to the list of devices requiring IP addresses. IP addresses must be assigned to GCs using a BOOTP Server. A BOOTP Server lists Ethernet addresses (which are unique to the communication card in each GC) and the IP addresses to be assigned to the corresponding device.

NOTE: For 450-GC only

To enable BOOTP Mode, follow these steps:

1. Locate the DHCP/Fixed IP switch behind the GC.
2. Switch to DHCP.

To edit IP addresses, follow these steps:

1. Obtain the Ethernet address for each GC from the GC front panel or the label on the Ethernet card.
2. Turn on the GC and press any key on the GC keypad to allow it to start in local mode. The Ethernet addresses are automatically loaded into the BOOTP Server list for GCs.
3. After the GC has completed its initialization process, press the button showing a tools graphic (i.e. wrench) on the GC keypad.
4. Press **Setup** on the keypad.
5. Press the **System** tab on the keypad.
6. Press **Change**.
7. In the Change network setting dialog box, press the IP address on the keypad.

NOTE: A stylus is located below the keypad for your convenience.

8. Press the corresponding numbers on the keypad to enter the IP address.
9. Press **OK** to save network settings.
10. Press **OK** to return to Home.

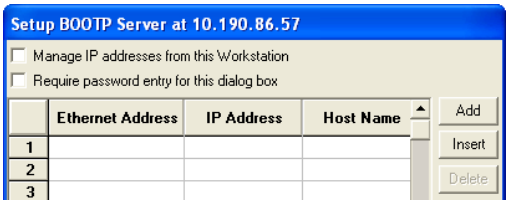
The GC Ethernet address automatically appears if the BOOTP Server is automatically updated by network devices.

NOTE: The BOOTP Server is updated less frequently over time by network devices. The BOOTP Server may not receive an update for up to a minute from any given GC.

11. After entering the Ethernet address for each networked GC into the BOOTP Server, power off the GC and then power on again.

12. Check that the IP address displayed on the front panel of each GC (in the Remote/Local Control screen) matches the intended address entered into the BOOTP Server. If they do not match, verify the Ethernet address, updating the BOOTP Server if necessary. Powering the GC off and on updates the IP address.

NOTE: If IP addresses are managed from a central location by a Network Administrator, then the BOOTP Server on your workstation must be disabled. Verify that Manage IP addresses from this Workstation is unchecked in the Setup BOOTP Server dialog box.



Using a Password to Protect BOOTP Settings

To restrict access to the **BOOTP Server**, which avoids inadvertent or unauthorized changes to IP address assignments, enable password protection in the **BOOTP Server** dialog box.

1. If the Setup Ethernet Ports dialog box is not displayed, select the **Setup Ethernet Communications** menu item from the **Instrument** menu to display the Communication Wizard.
2. Click **Next** to advance to the **Setup Ethernet Ports** dialog box.
3. Click **Setup.**
4. Check Require password entry for this dialog.

The next time you enter the BOOTP Server from the Setup Ethernet window, you are prompted for a password.

After you successfully enter a password, you may change it. Enter a new password twice.

The initial password is blank (no password). To set your password initially, enter the desired password in the Enter new password and Re-enter new password fields.

Enter the password each time you open the BOOTP Server.

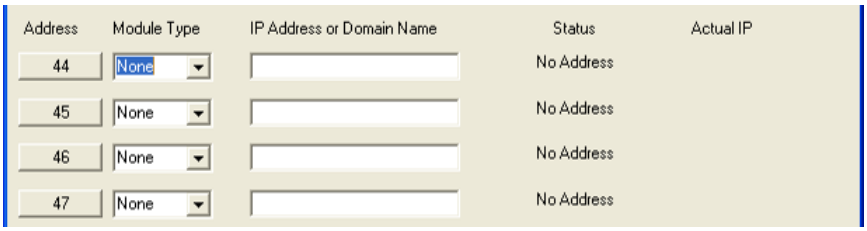
NOTE: Refer to *Recovering a Lost Password for BOOTP Server Access* in the *Diagnostics/Troubleshooting* section for instructions on resetting the password.

Adding a GC and MS in System Control

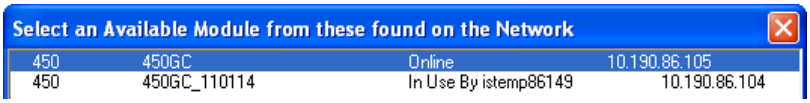
After configuring the Workstation computer and GC for network communication, select a GC to be controlled from each MS Workstation.

If it is not already running, start System Control. The Communication Configuration Wizard will open if you have not yet configured your GC Ethernet connections.

1. Click **Next** to advance to the **Setup Ethernet Ports** dialog box.
2. Click the **Address** for a GC.



3. Click the GC to connect and click **OK**. This example uses a 450-GC.



NOTE: If you are running on a company network, only GCs on the same local subnet appear in the Select Available Modules dialog box. To connect to a GC in a different subnet, type its IP Address directly into the IP address field in the Setup Ethernet Ports dialog box. Consult your Network Administrator about subnets on your network.

4. The **Setup Ethernet Ports** Dialog Box shows the GC connected to the Workstation. In this example a 450-GC is connected to Port 44. Status shows the GC is online and the IP address of the GC displayed. Click **OK**, and wait for the GC to connect.

After the GC connects to System Control, a GC icon appears at the bottom of the **Configuration Window**. The icon is labeled 450-GC.44, and includes the Host Name of the GC appended to the label. The number 44 is a System Control communication address.

Modules and Instruments

The 210-MS Ion Trap Mass Spectrometer is paired with a 431-GC Gas Chromatograph. The 220-MS or the 225-MS Ion Trap Mass Spectrometer is typically paired with a 450-GC Gas Chromatograph. The Combi PAL AutoSampler is another possible module.

NOTE: While the CP-8400 and CP-8410 AutoSamplers do not have separate icons, they are included on the GC Status and Control Window.

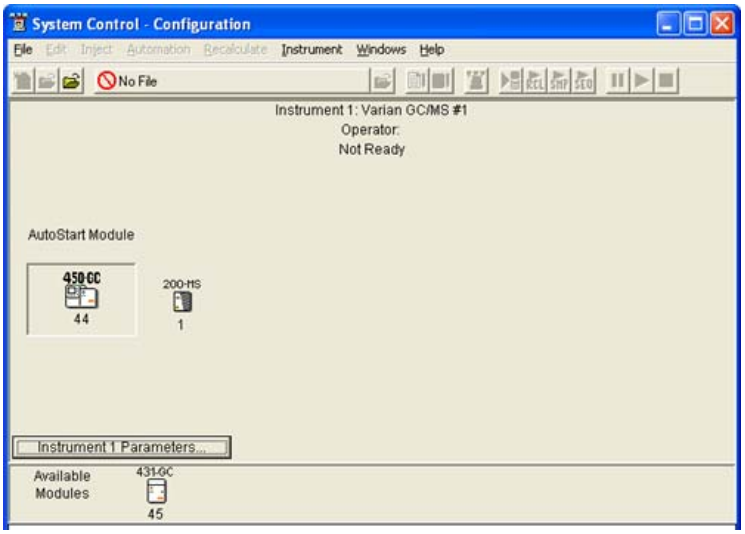
These modules also have addresses and the message logs frequently refer to them. The modules and allowed addresses are listed on the following table.

Module	Name	Address
Mass Spectrometer	220-MS	56
Gas Chromatograph	450-GC	44
AutoSampler	Combi PAL	24

NOTE: The Workstation, module name for the 210-MS, the 220-MS, and the 225-MS is 200-MS.

Elements of the Configuration Screen

After the GC connects to **System Control**, configure it as an Instrument by moving its icon from the Available Modules of the Configuration Window into the Instrument Area.

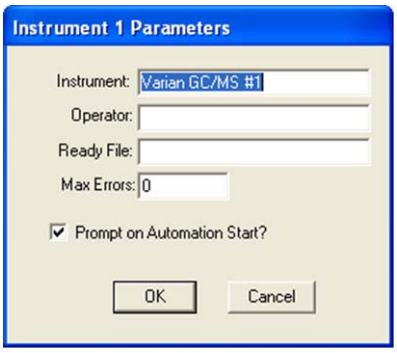


Configure each module the same.

Place the GC icon in the AutoStart Module window if either a CP-8400 or CP-8410 AutoSampler are used with the GC. If a Combi PAL is used, place the Combi PAL icon inside the AutoStart Module window. If the GC operates without an AutoSampler controlled from the Varian MS Workstation, leave the AutoStart Module box empty. If you are using a sampling device, the device must be connected to the synchronization port of the GC.

Setting Instrument Parameters

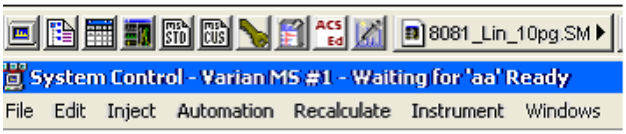
Use the Instrument Parameters to enter information such as the description of the Instrument, Operator's name, and Max Errors.



The instrument name appears in the instrument window. The instrument and operator names appear on any automated reports generated by MS Workstation. The Ready File is not used with MS Workstation Version 6.

When the maximum number of non-fatal errors (Max Errors) is exceeded during automation, the automation sequence halts. Setting this value to zero disables this feature. You are optionally prompted for this information when you start an automated sequence of injections or Recalculations. If the Prompt on Automation Start box is checked, this dialog will appear when an Automation is started. This feature can be particularly useful if different operators use the GC/MS instrument.

NOTE: Do not enter any characters in the Ready File field or the MS will not come to Ready for injections. For example, if the characters **aa** were entered in the Ready File field, the System Control title bar would contain the "Waiting for 'aa' Ready" warning as displayed here. Even an invisible space character in this field can cause the problem.



Running an MS Method without a GC Method

To run an MS method without the GC module or GC method.

1. Open **System Control**.
2. Select **Configuration** from the **Instrument** menu.
3. Click and drag the GC icon, and AutoSampler icon, if present, from the middle field to below the bar labeled Available Modules.

When an MS method is activated, the GC method will not be downloaded. To activate the GC and AutoSampler modules, click-drag-drop the icons into the active field.

Using MS Workstation Toolbar

Overview

MS Workstation is a suite of applications for controlling chromatographs, collecting data from chromatograph detectors, and analyzing those data. The MS Workstation Toolbar provides quick and easy access to the MS Workstation applications. When activated, the MS Workstation Toolbar behaves very much like the Windows Taskbar. It docks on any of the four sides of the display screen and other Windows programs will not cover or go behind it when they are opened in full screen mode.

To open the Workstation Toolbar from Windows Desktop, follow these steps.

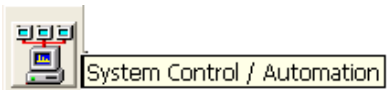
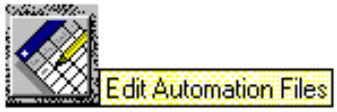
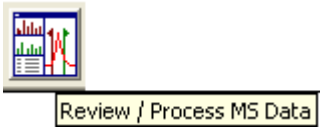
1. Click the **Start** button.
2. Click **All Programs**.
3. Click **MS Workstation**.
4. Click **Workstation Toolbar**.

Toolbar Applications

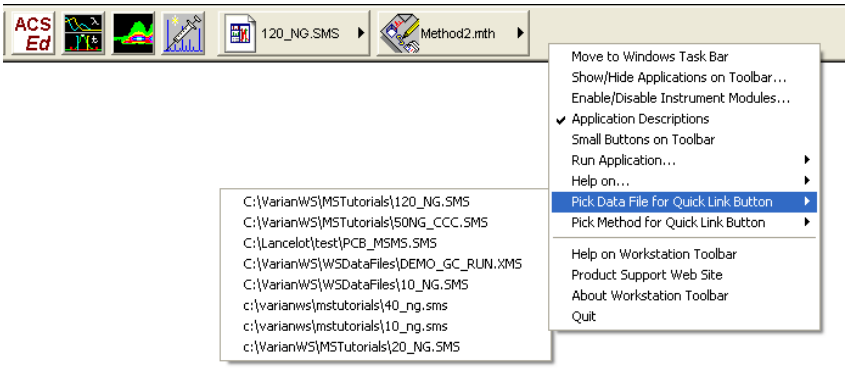
The toolbar provides application buttons.

- Tooltips show the application name when the cursor rests on the Application Button.
- Quick Link Buttons provide a menu to be performed on the listed file.
- Application Descriptions give a brief description of the application that open when the cursor rests on the Application Button.

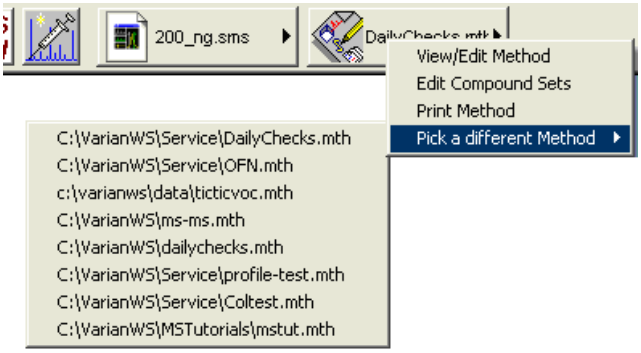
Application Buttons

	Monitor instrument status, perform automated injections, and perform batch recalculations.
	View and edit instrument operation, data acquisition, and data handling methods.
	Edit SampleLists, RecalcLists and Sequences off-line.
	Review chromatograms and spectra, perform library searches, and review and process quantitation results.
	Create, edit, and view standard MS reports.
	Create, edit, and view customized MS reports.
	Convert data files between DOS and Windows formats.
	Review standard GC chromatograms, interactively edit data handling parameters, and recalculate results.
	Preview standard chromatogram and results reports.
	Generate standard reports for a group of Data Files by dragging and dropping them on the Batch Report Window.
	Run a sample without a Sample List.
	Set MS Workstation security options and passwords.

Quick Link Buttons



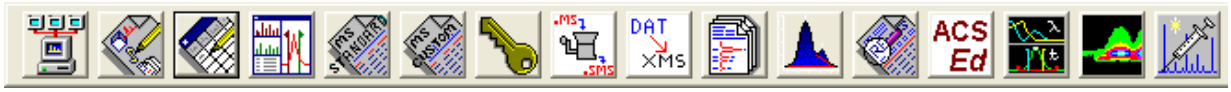
Most Recently Used Data File. Menu for the Most Recently Used Data File. Select a different data file from a list of most recently used files.



Most Recently Used Method. Menu for the Most Recently Used Method. Select a different method from a list of most recently used methods.

Toolbar Applications

Icon for the Applications



MS Workstation applications are icon buttons on the MS Workstation Toolbar. As you move the mouse over these buttons, the name of the application is displayed in a tooltip window below the cursor.

Click an icon in the MS Workstation Toolbar to launch application.

Data File and Method Quick Link Buttons

The two buttons to the right of the application buttons are Quick Link buttons. These two Quick Link buttons correspond to recently used Data Files and Methods. On each Quick Link button is the name of the file associated with that button. When you click the Quick Link button, a menu is displayed showing operations that can be performed on the corresponding file.

The Quick Link buttons in the MS Workstation Toolbar are updated with the most recently used Data File and Method. If the Data File or Method you need is not displayed in the Quick Link button, choose from the eight most recently used files by selecting “Pick a different Data File (or Method)” from the Quick Link button’s menu.

Toolbar Options

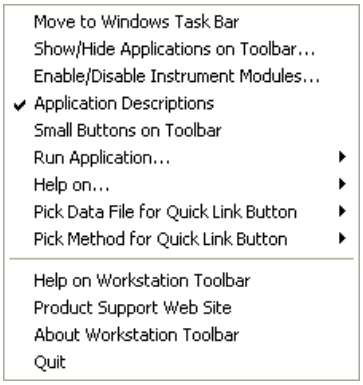
Moving the Toolbar

The MS Workstation Toolbar can be moved to any edge of the Windows screen. Click a portion of the MS Workstation Toolbar that does not contain application or Quick Link buttons and drag the toolbar to the edge of the screen that you desire. When you release the mouse, the toolbar will remain on that edge. The MS Workstation Toolbar remembers its location the next time it is started.

Additionally, display the MS Workstation Toolbar as a Windows Taskbar icon. To do so, select “Move to Windows Taskbar” from the MS Workstation Toolbar options menu. Taskbar icons appear in the lower right (or bottom) of the Windows Taskbar (the bar on which the “Start” button appears). When displayed as a Taskbar icon, the toolbar no longer takes up space on the screen. When you click the MS Workstation Toolbar icon, the options menu is displayed.

Toolbar Options Menu

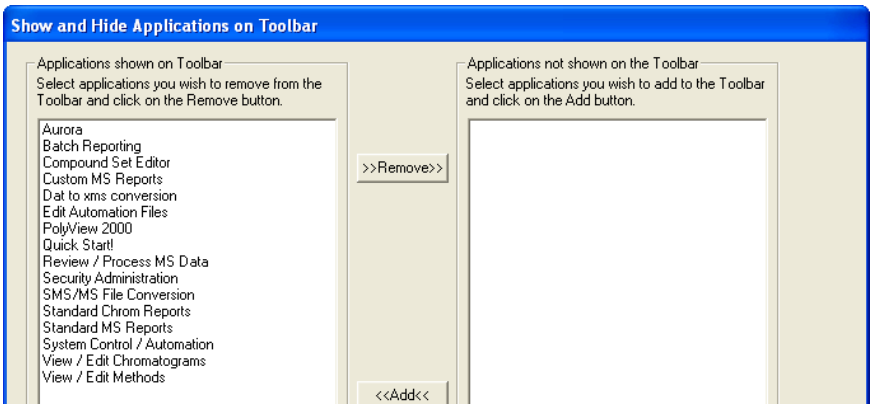
Move the mouse over an area of the MS Workstation Toolbar not containing application or QuickLink buttons, and right-click to display an option menu.



Move to Windows TaskBar

Display the MS Workstation Toolbar as a Windows Taskbar icon. Taskbar icons appear in the lower right (or bottom) of the Windows Taskbar (the bar on which the “Start” button appears). When displayed as a Taskbar icon, the toolbar no longer takes up space on the screen. When you click the MS Workstation Toolbar icon, the options menu is displayed.

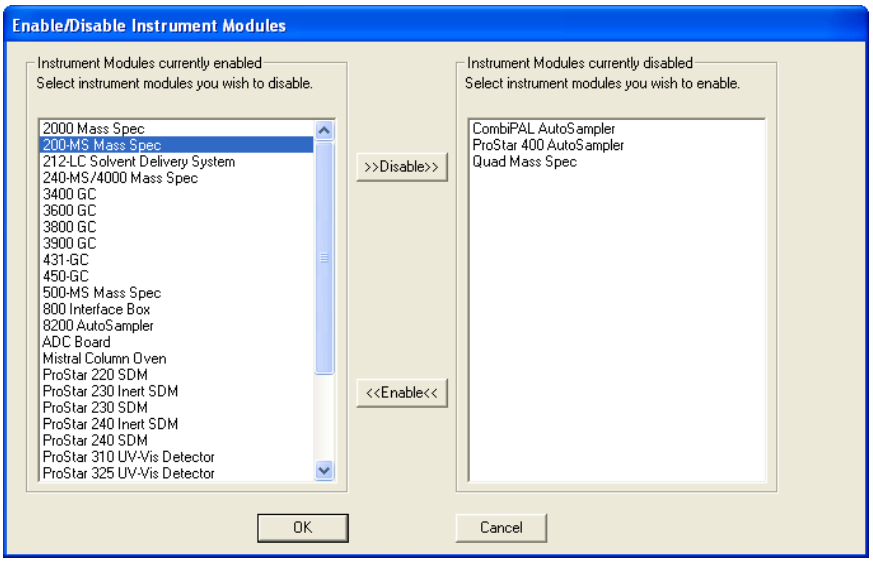
Show/Hide Applications on Toolbar



Select which MS Workstation applications are represented by icons on the MS Workstation Toolbar. The right list box shows all applications that are currently displayed in the toolbar. The left list shows all applications that are installed but not displayed in the toolbar.

Enable/Disable Instrument Modules

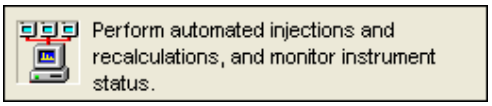
Display the Enable/Disable Instrument Modules dialog box.



Select the MS Workstation instrument modules available from the workstation. When an instrument module is available, it appears in System Control if the corresponding instrument is connected and on. You can create a Method section for it and format reports.

The left list box shows instrument modules that are currently installed and enabled in MS Workstation. The right list shows instrument modules that are installed but not enabled.

Application Descriptions



Check this to display descriptions when you move the mouse over application buttons in the MS Workstation Toolbar.

Small Buttons on Toolbar

Select this to display a smaller MS Workstation Toolbar. The icon for an application may change.

Run Application

This lists all applications showing on the MS Workstation Toolbar. Click an application to launch it.

Help on

This lists all applications showing on the MS Workstation Toolbar. Eelect an item from this list, to display the online help.

Pick Data File for Quick Link Button

This lists the eight most recently used Data Files in order of use. Select a Data File from this list to display it in the Quick Link button.

Pick Method for Quick Link Button

This lists the eight most recently used Methods in order of use. Select a Method from this list to display it in the Quick Link button is.

Help on MS Workstation Toolbar

Displays the help you are using.

Product Support Web Site

If you have Internet access and a web browser installed on your computer, this option ill automatically opens theVarian Product Support Web Site. This site has the latest software and documentation updates for the Varian suite of products, along with additional notes, tips, and answers to frequently asked questions.

Visit this site periodically to see if new information and relevant information.

About MS Workstation Toolbar

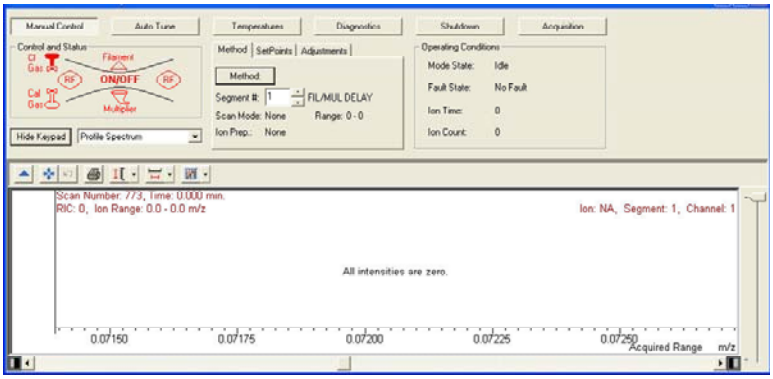
Displays the About Box for the MS Workstation Toolbar. The About Box contains information about the software version, installation information, and a list of the instrument control modules that are installed.

Quit

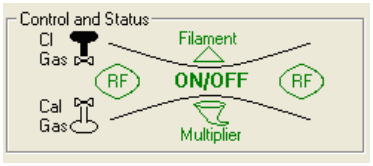
Quits the MS Workstation Toolbar application. If you run the MS Workstation Toolbar automatically when Windows starts, the MS Workstation Toolbar opens the next time you start Windows.

Controlling the MS

The MS Module Window is similar to the following. If you do not see this screen, go to the menu labeled Instrument, and click GC/MS.

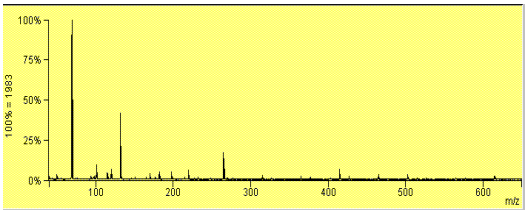


The upper left side of the window has the ion trap schematic, which turns the ion trap on. If the trap is displayed in red, it is disabled. The trap is disabled if the current segment is a filament/multiplier delay segment, one with an ionization mode of none, or if a fault has occurred. If the ion trap icon is not currently disabled, clicking in the center of the ion trap turns on the trap. The black schematic turns green to show that it is on.

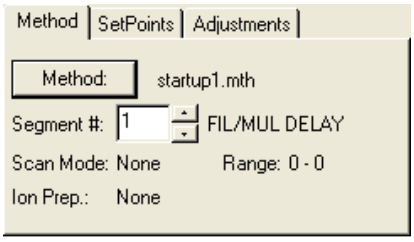


Select a method segment that is not a Filament/multiplier delay segment to enable the ion trap. The method and segment selection is in the center of the screen and has the active method and the instrument set points.

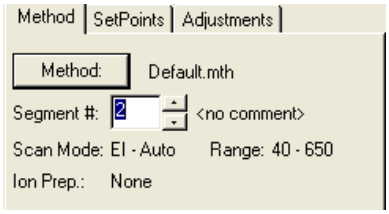
The ion trap symbol shows the endcaps (two horizontal curved lines), the rf-voltage ring electrode (two vertical curved lines), the electron multiplier (a curved cone), the filament (a triangle), the tank for the CI reagent gas, and the reservoir for the calibration compound. Click the appropriate part of the ion trap symbol, or click the corresponding button, to turn on and off the parameters in the symbol (i.e. click triangle to turn on filament). Click in the center of the trap and the Cal Gas bulb, to display a spectrum of PFTBA.



Method



The Systme Module has three tabs; Method, SetPoints and Adjustments. The active method always controlls the GC/MS system. This method is the last method selected from a previous use or the default method if the instrument is just being configured. In the default method, the first MS Method Segment defines a Filament/Multiplier Delay. When this segment is active, the trap controls are off and no scans are taken to protect the trap from solvent peaks that elute shortly after injection. Specify this segment is specified by selecting an Ionization Mode of "None." When this segment is active in Manual Control, the trap icon appears red, indicating that the trap is off and that its state cannot be changed. To take and display scans, select an MS Segment with an Ionization Mode of other than None. The trap icon returns to black. Below the method button is the segment number.

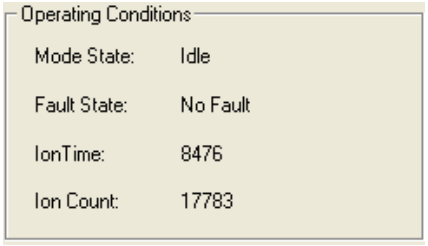


The fields are from the method in use.

- Scan Mode describes the ionization mode of the current segment, for example, EI-Auto.
- Ion Prep. is the ion preparation method of the current segment, such as MS/MS.
- Range shows the mass range being scanned by the current segment.

Operating Conditions

Operating Conditions displays the current instrument information on the far left of the MS Module window.

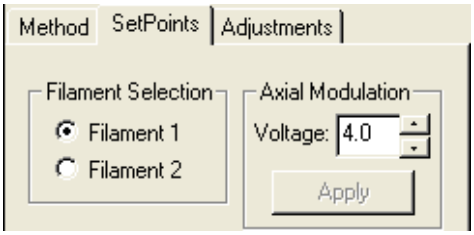


- Mode State indicates the function the MS is performing.
- Fault State indicates a fault has occurred.

- Ion Time indicates the ionization time of the last scan.
- Ion Count indicates the ion count of the last scan. If profile mode is selected, this is the total ion count. If centroid mode is selected, this is the reconstructed ion count.

SetPoints

Use the SetPoints tab to select the filament and the axial modulation voltage.



The two filaments reduce down time for maintenance. Select the filament.

The Axial Modulation Voltage is applied to the endcap electrodes.This voltage is critical to resolution and sensitivity. In most cases, the best Axial Modulation voltage is the lowest value at which there is still good resolution of the 131/132 and 414/415 cal gas peaks. For most instruments this value is between 2 and 4 volts.

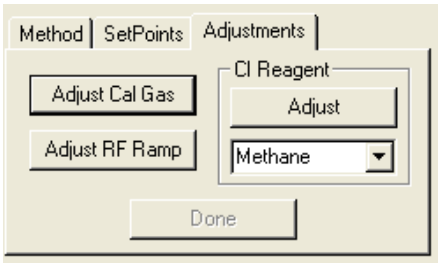
Adjust the Axial Modulation voltage before determining the Automatic Gain Control (AGC) target TIC and before performing the mass calibration.

If the value of the Axial Modulation voltage is too low, high molecular weight ions will not be observed. If the value for the Axial Modulation voltage is too high, the widths of the peaks of low molecular weight ions will be broadened and mass misassignments may occur.

NOTE: Mass calibration must be redone if the axial modulation setting is changed.

Adjustments

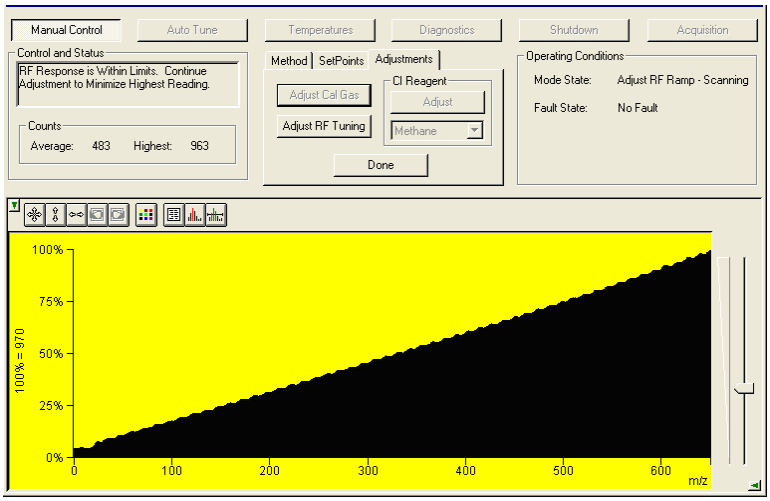
The third tab is the Adjustments tab.



This tab adjusts the Cal Gas pressure, the CI Reagent gas pressure, and the RF Ramp. Also, select the CI reagent.

Adjust RF Ramp

Click **Adjust RF Ramp** to determine if the RF voltage is in tune throughout the entire mass range of the MS by observing the RF modulator response.



The rf Modulator Response screen shows a real time view of the rf modulator response from 20 to 650 m/z. The vertical axis of the display is in percentage of counts, and the horizontal axis is mass units. One scan, over the entire mass range, requires about 1s.

The counts are displayed as Average rf modulator response and Highest rf modulator response.

To monitor the rf voltage, observe the ramp. If the rf voltage generator circuit is properly tuned, the ramp will rise gradually in a straight line from low mass to high mass without any sudden rises in the ramp, and the Average number counts are less than 1000. If the rf voltage generator is not tuned properly all the way to 650 m/z, the end of the ramp rises sharply at the mass above which the generator is out of tune, and the Average number of counts might be above 1000. If so, adjust the rf voltage.

The text to the left of the rf button states if an adjustment is necessary.

- If the rf voltage is tuned throughout the entire mass range, the following is displayed:

  rf response within limits
  continue adjustment to minimize highest reading

- If the rf voltage is out of tune, the following is displayed:

  rf response out of range adjust the rf screw
  for a linear response

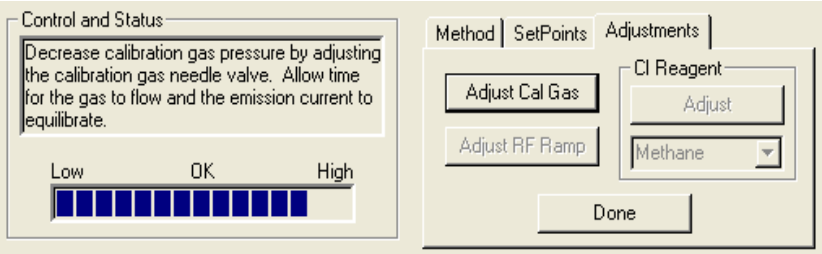
Tune the rf coil by adjusting its resonant frequency to match that of the output of the rf generator board. This is done as follows.

1. Open the front door and insert a flat head screwdriver into the tuning rod in the hole labeled “RF ADJUSTMENT” on the lower part of the front panel.
2. Slowly turn the screw clockwise until the slope of the ramp increases, then turn the screw counterclockwise until either the slope of the ramp is at its lowest or there is a sudden rise at the end of the ramp.

3. Turn the screw three turns clockwise and verify that the Average number of counts is less than 750 and the Highest number of counts is less than 1500. If they are, the coil is successfully adjusted. If not, run Diagnostics and call a qualified service representative.
4. When it is properly adjusted, the dialog states the rf response is within limits.
5. When you are finished, click the Done button.

Adjust Cal Gas

To adjust the Cal gas pressure click **Adjust Cal Gas**.



Adjusting the cal gas has the following actions. The filament, electron multiplier, and rf voltage are turned on; the calibration compound solenoid operated valve is opened; and the scan range is set to display calibration compound peaks from 45 to 135 m/z. The program determines if the calibration compound pressure in the vacuum manifold is too low, too high, or satisfactory.

The Control and Status dialog box displays messages that indicate the status of the calibration compound pressure in the vacuum manifold. The messages are listed.

Below the dialog box, a progress bar display that shows the status of the pressure visually.

If the pressure is satisfactory, the following message is displayed:

The calibration gas pressure is OK. Allow time for the gas to flow and the emission current to equilibrate.

If so, click **Done**.

If the calibration compound pressure is too low, the following message is displayed:

Increase calibration gas pressure by adjusting the calibration needle valve. Allow time for the gas to flow and the emission current to equilibrate.

If so, turn the calibration compound needle valve 1/4 turn counterclockwise. Wait for about 30 seconds for the instrument to equilibrate. Then, note the message again.

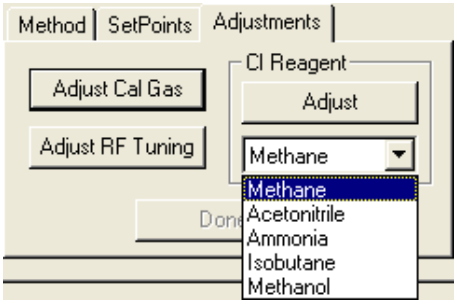
If the pressure is too high, the following message is displayed:

Decrease calibration gas pressure by adjusting the calibration needle valve. Allow time for the gas to flow and the emission current to equilibrate.

If so, turn the calibration compound needle valve 1/4 turn clockwise. Wait for about 30 seconds for the instrument to equilibrate. Then, note the message again.

CI Reagent (Adjust)

To use Chemical Ionization, select a CI reagent gas and adjust its pressure. Select the reagent gas from the menu below the word Adjust.



In CI, as in EI, the MS is tuned to achieve the best combination of maximum peak height (sensitivity), optimum resolution of peaks, and smooth peak shape. The key to proper tuning is to optimize the number of ions in the ion trap: If there are too few ions, sensitivity suffers; if there are too many ions, resolution and peak shape suffer.

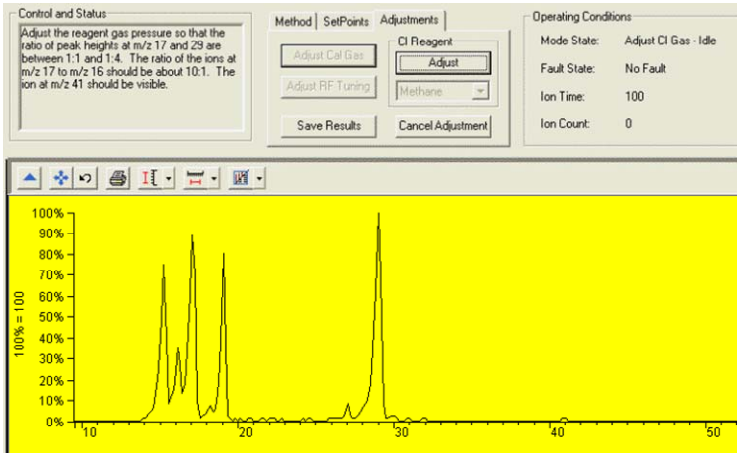
In CI, the two main factors that affect the number of ions in the ion trap are the ionization time and the reaction time. the emission current is an important third factor.

The CI ionization time is the time that energetic electrons, emitted from the filament, interact with reagent gas to form reagent ions. The reaction time is the time that reagent gas react with sample molecules to form ions.

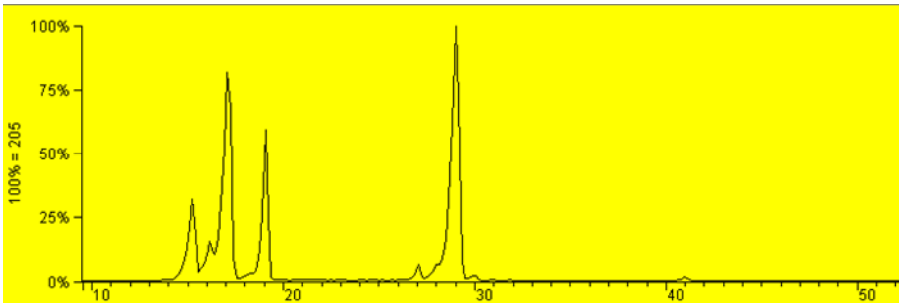
The number of reagent ions formed is directly proportional to the ionization time, and the number of sample ions formed is directly proportional to the reaction time.

After selecting methane as the CI reagent gas, adjust the flow rate of the gas into the mass spectrometer by doing the following.

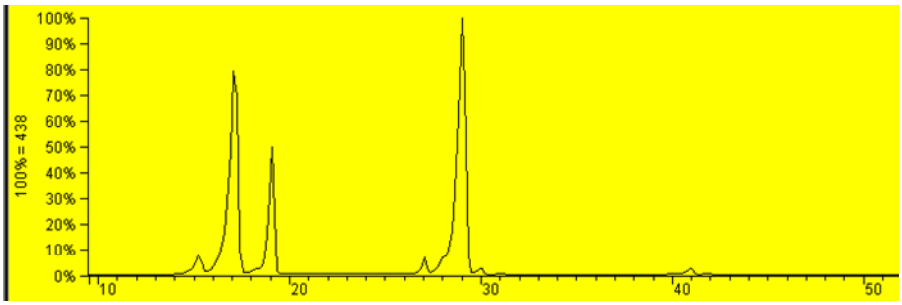
1. Make sure that the gas tank is open and connected to the back of the instrument.
2. Click Adjust to open the CI valves; turn on the filament and multiplier. The following is an example of the CI gas spectrum for methane, in which the CI gas pressure is too low. Notice the resolution and relative ratio between masses 10 and 30.



1. Increase the CI gas pressure by adjusting the CI needle valve on the front of the MS. Turn the knob clockwise to increase the pressure. In the following spectrum the pressure is correct.



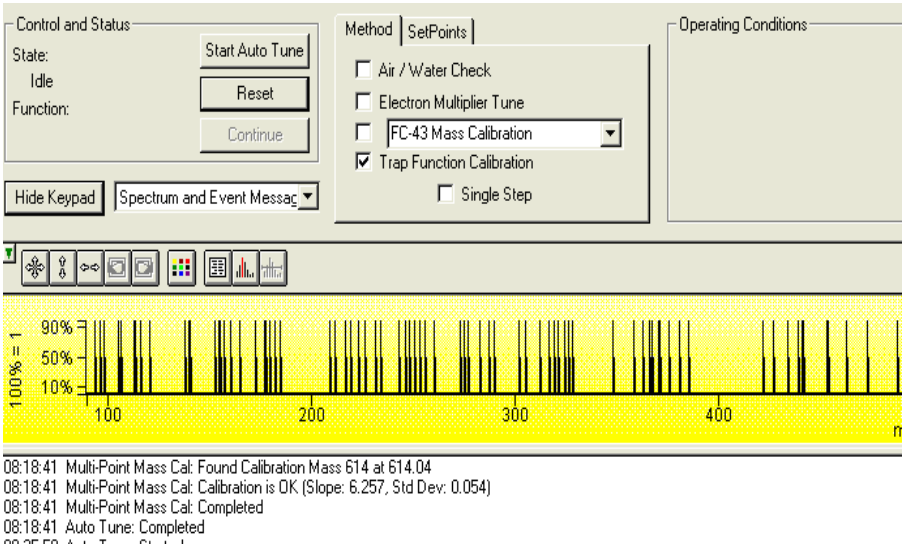
2. If the pressure increase is too much, a spectrum like the following is displayed.



Auto Tune Mode

Recalibrate the mass axis (FC-43 Mass Calibration) whenever the temperature, axial modulation, or rf adjustment is changed. Each time the system is shut down, perform auto tune after restarting it.

The Auto Tune window has four sections: the Control and Status, Method and Set Points, Operating Conditions and the Spectrum and Event Messages.

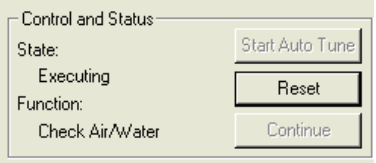


Control and Status

Start Auto Tune by clicking **Start Auto Tune**. Stop AutoTune by clicking **Reset**.

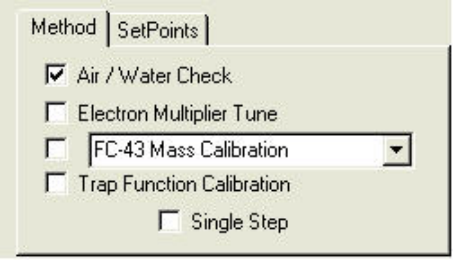
State displays if the MS is executing an auto tune function or idle.

Function shows which tuning function is being performed.

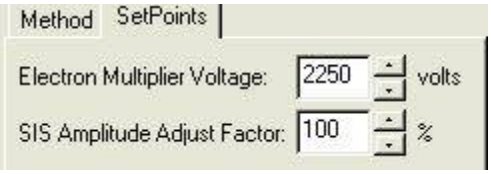


Method and SetPoints

There are four procedures that set up, tune and calibrate the mass spectrometer. Air/Water check, Electron Multiplier Tune, Mass Calibration and Trap Function Calibration.



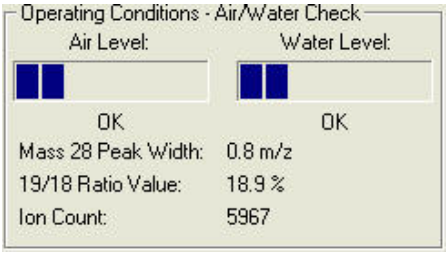
Use Set Points to manual adjust the Electron Multiplier Voltage, and the Selected Ion Storage (SIS) Amplitude Adjust Factor.



NOTE: The Air/Water Check uses the last 10^5 Electron Multiplier Setting and not the manual setting. If the electron multiplier is replaced, autotune the Electron Multiplier Tune before doing the Air/Water Check.

Operating Conditions

The display shows the status of the inprogress procedure.

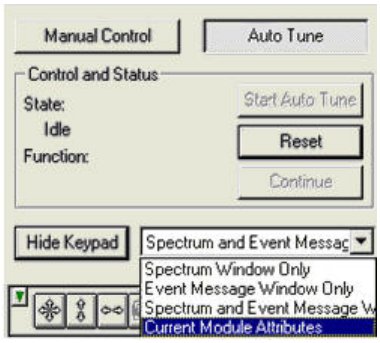


Use the width of the mass 28 peak width is to determine if air is present in the trap. The progress bar Air Level represents the peak width.

Use the mass 19/18 ratio to determine if water is present. The progress bar Water Level" represents the ratio.

Spectrum and Event Message Window

Select the information to display during the auto tune tests by clicking the arrow and selecting from the display options. The Hide Keypad button hides the upper portion of the screen and expands the lower portion.

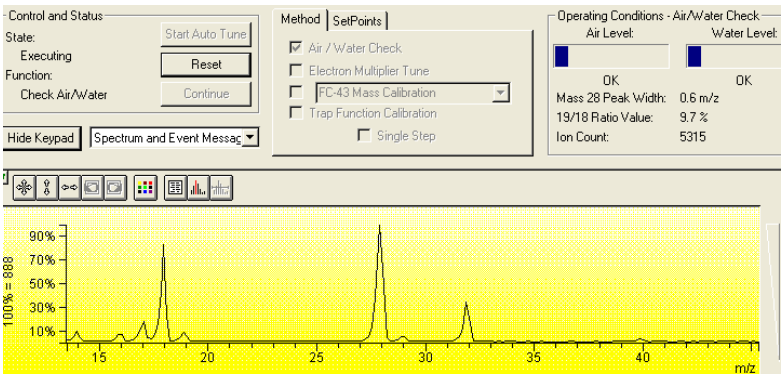


Current Module Attributes is the information stored from the last auto tune. After finishing an auto tune, view this information as an auto tune log.

```
Setpoints
        Trap Temperature:                       150 degrees C
        Manifold Temperature:                    35 degrees C
        Transfer Line Temperature:              170 degrees C
        Filament Number:                          1
        Axial Modulation Voltage:               5.0 volts
Air/Water Check
        Last Checked:                   7/15/98 10:52 AM
        Air Level Test Result:           OK
        Water Level Test Result:         OK
        Mass 28 Peak Width:                0.6 m/z
        Mass 19 to Mass 18 Ratio:         10.1%
        Total Ion Count:                  3594 counts
Integrator Zero Set
        Last Executed:                  7/15/98 7:05 AM
        Integrator Zero Set Result:     OK
        DAC Setpoint:                      120 DACs
        Average Counts:                    0.5 counts
```

Auto Tune Checks

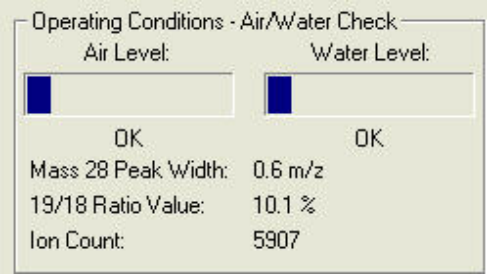
The top center has four check boxes. These are the auto tune steps. To perform the auto tune click the check boxes and click Start Auto Tune.



Each selected procedure is executed. If you checked the single procedure, only that procedure is performed. Stop auto tune by clicking Reset.

Air/Water Check

When Air/Water Check is in process, you can determine the relative amount of air and water vapor in the vacuum manifold from the display. The following happens automatically: The filament, electron multiplier, and rf voltage are turned on; AGC is turned off; and the scan range is set to display the air/water spectrum (14 to 44 m/z). To determine the air background, the width of the peak for mass 28 at 10% peak height is calculated. To determine the water background, the ratio of mass 19 to mass 18 is calculated.



The left side has a progress bar that indicates the relative amount of air in the system. A message is displayed below the bar.

If the display reads OK, there is essentially no air leak in the system. If the message MAYBE is displayed, there is a small air leak. The system can be operated, but performance might not be optimum.

If the display reads HIGH, there is a significant air leak. The leak must be found and corrected before the system can be operated.

The right side has a progress bar that indicates the relative amount of WATER in the system. A message is displayed below the bar.

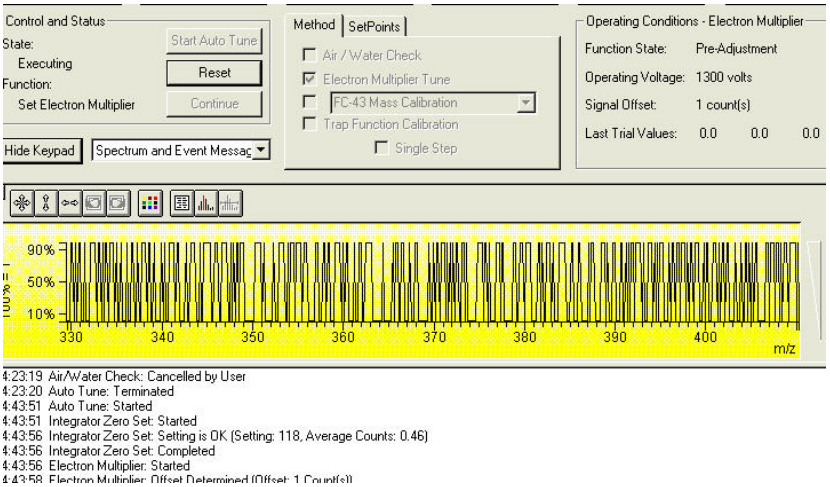
If the meter reads OK, there is very little water and the system can be operated.

If the display reads MAYBE, there is a small amount of water, and the system can be operated, but performance might not be optimum.

If the meter reads HIGH, there is a comparatively large amount of water present in the system, and the system must be baked out to remove the water before the system can be operated. (A relatively high water background is generally observed immediately after you have vented the instrument. It will usually go away within a few hours of restoring the instrument to its normal operating conditions.)

NOTE: The Air/Water Check uses the electron multiplier voltage with a 10^5 gain and not the manual setting. If the electron multiplier is replaced, the autotune of Electron Multiplier Tune must be done *before* the Air/Water Check.

Electron Multiplier Tune



The Electron Multiplier Tune determines three proper settings: the Integrator Zero, the 10^5 gain for the Electron Multiplier, and the Electron Multiplier voltage boost for optimum peak intensity and resolution.

The Integrator Zero Set obtains the average value of the signal level coming from the Integrator Circuitry when the filament is off. When the filament is off, the major source of signal coming from this circuitry is electronic noise. The Integrator zero is adjusted so that the average value of electronic noise is slightly greater than zero.

NOTE: The average value for the integrator zero must between 0.20 and 0.80 counts. The setting can range between 0 and 255.

The Electron Multiplier Tune program can automatically set the electron multiplier voltage, such that the electron multiplier gain is approximately 10^5 electrons per ion. Run this only when there is no sample in the instrument. For example, wait at least 30 minutes after you close the calibration compound valve before running the program.

For the determination of 10^5 gain, Electron Multiplier Tune program runs in two phases. In the first phase, the electron multiplier is set to a low test voltage, the message PRE-ADJUSTMENT PHASE is displayed. The electron multiplier voltage is increased by 100V increments until a signal is detected coming from the electron multiplier. The electron multiplier voltage is then set to 300V less than the value at which a signal was first detected.

In the second phase, the electron multiplier voltage is increased by 100V increments beginning with the final value of the first phase of the program. In this phase, the Locate Low Voltage End where 10^5 gain is not achieved and Locate High Voltage Start where 10^5 gain is exceeded are determined.

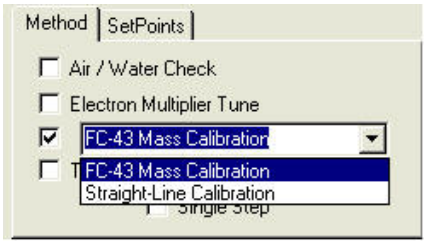
NOTE: The electron multiplier is approaching the end of its lifetime when the voltage setting nears 3000 volts.

The final determination is the Electron Multiplier boost, which determines the EM voltage and AGC Target value for optimum peak intensity and resolution. It uses the calibration compound peak at mass 131. The program adjusts the target TIC value to a level that provides reasonable resolution of the major peak and its first

isotope peak. The program determines the height and area of the major peak of interest, the height and area of the isotope peak, the height of the valley between the two peaks, and ratio of the height of the valley and the height of the isotope peak. The Final Gain setting reflects any increase in the voltage for optimal sensitivity and resolution. This setting is also the value displayed in the Set Points dialog, which is in the Electron Multiplier voltage field.

Mass Calibration

The mass calibration function adjusts the rf scale for a coarse full mass range calibration and, then locates several FC-43 masses for a multi-point calibration curve.



To perform mass calibration based on FC-43, select the checkbox to the left of FC-43 Calibration.The calibration compound valve opens, and the electron multiplier, filament, and rf voltage are turned on. The program uses the calibration compound peaks at masses 69, 131, 264, 414, 464, 502, and 614 to create a calibration curve.

Factors Affecting Mass Calibration:

- The program uses the air peak at mass 28 for the calibration of low masses. Air leaks result distort low mass calibration. Do not run the Mass Calibration program if your instrument has an air leak.
- If one or more of the mass peaks are not found by the program, check and if needed, adjuist the rf voltage amplitude.
- Temperature changes can adversely affect the mass calibration. Start this procedure after the manifold has reached its equilibrium point (approximately 3 hours after the set-point temperature has been established).

An ideal slope is 6.300 steps per atomic mass unit. The acceptable range for is 6.3 ± 0.1. The standard deviation must be 0.15 steps per atomic mass unit or less. (If your standard deviation is outside of these limits, check the rf voltage amplitude over the entire mass range).

Straight Line Mass Calibration

Click Straight Line Calibration and Start Auto Tune. A straight line calibration assumes a linear relationship between DAC steps and mass. It is used for some hardware adjustments. When initiated, a straight line calibration curve is calculated with the zero DAC step set equal to 0 m/z and 4095th DAC step set equal to 650 m/z.

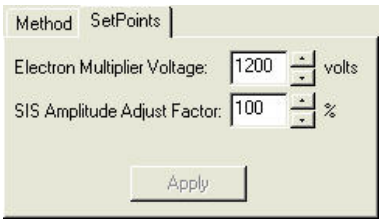
Trap Function Calibration

After completing mass calibration, perform trap function calibration. This determines the parameters that are required to operate ion preparation methods such as MS/MS and SIS. It takes several minutes to complete. Perform Trap Function calibration each time a mass calibration is done**.** If ion preparation methods are not in use, the trap function calibration is not needed. However, before activating an ion preparation method, repeat the mass calibration and a trap function calibration.

```
08:46:53  Auto Tune: Started
08:46:54  Trap Function Calib: Started
08:46:59  Trap Function Calib: Calibrating at Mass 69
08:48:39  Trap Function Calib: Calibrating at Mass 131
08:50:27  Trap Function Calib: Mass 69 Calibrated (Freq: 258.050 kHz)
08:50:28  Trap Function Calib: Mass 131 Calibrated (Freq: 255.300 kHz)
08:50:28  Trap Function Calib: Completed
```

At the end of Trap Function Calibration, the Event Message Window displays the frequency values for the two trap function calibration points. Nominal values are 257 and 255, respectively. These values can vary up to ± 4 KHz between instruments.

SetPoints



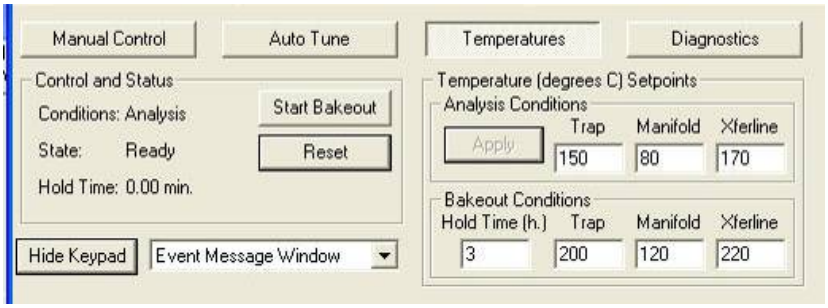
Set the electron multiplier voltage and the SIS amplitude adjust factor by either changing the value or by clicking the arrows. The values are not set until Apply is clicked and are reset to their previous values if Apply is not clicked.

Electron Multiplier Voltage. Final Gain Setting determine from the Auto Tune EM check.

SIS Amplitude Adjust Factor. Adjust for optimum ion sensitivity and ejection. The voltage adjustment factor may be set between 50 to 200%. The default is 100%.

Temperatures Mode

Click Temperature.



Click any temperature to change it. After changing a setting, click Apply.

Manifold temperature: range 0°C to 120°C; default = 40°C

Trap heater: range 0°C to 250°C; default = 150°C

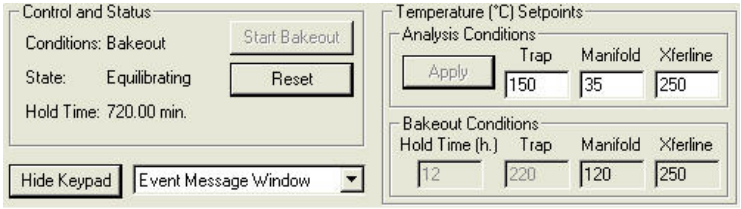
Transfer Line temperature: range 0°C to 350°C; default = 170°C.

The manifold heater bakes out the analyzer and should not exceed 50°C when acquiring data. The recommended default temperature is 40°C. Adjust the transfer line temperature so it not lower than the trap or the GC oven.

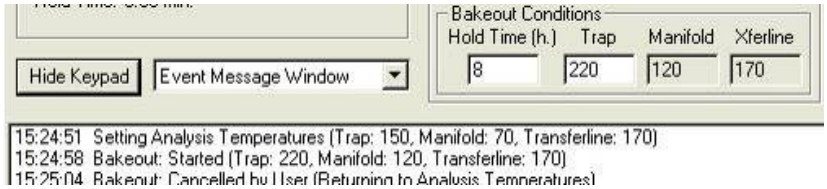
NOTE: DO NOT heat the transfer line above the maximum temperature specified for the capillary column.

After chaning a temperature, wait 2 to 3 hours to let the system equilibrate. After equilibrium is reached, check the rf tuning, and adjust if necessary.

Start Bakeout activates Bakeout Conditions (time and temperature). Reset ends the bakeout session. The manifold bakeout temperature is fixed at 120 °C. The transfer line bakeout temperature defaults to its Setpoint temperature.



After changes are performed, the event log at the bottom of the screen updates with the time and the event. The following is an example.

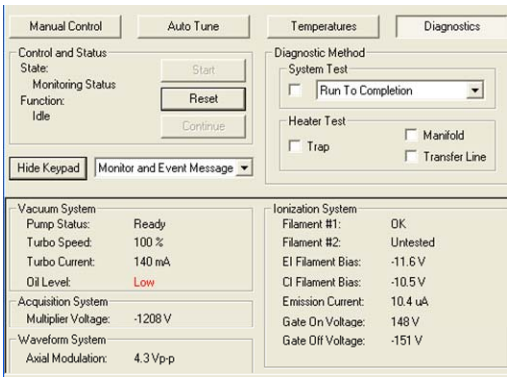


After bakeout, the trap, and manifold temperatures return to the set point values. New setpoint values can be applied during a bakeout. A bakeout must be halted, before a new bakeout duration or new bakeout temperatures can be set.

Diagnostics Mode

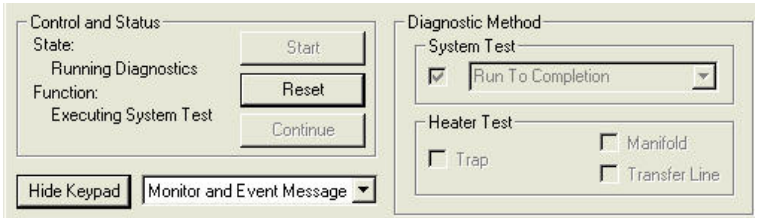
Monitoring diagnostics on startup helps to identifiy problems.

Click Diagnostics in the top center of the screen. The following is the diagnostic window of the 225-MS, which has an Oil Level readback.The window for the 210-MS and 220-MS is the same with the exception of the Oil Level readback



The upper portion of the screen has 3 sections: Control and Status, Diagnostic Method, and Monitor States.

Start an automated diagnostics by clicking Run to Completion and clicking Start



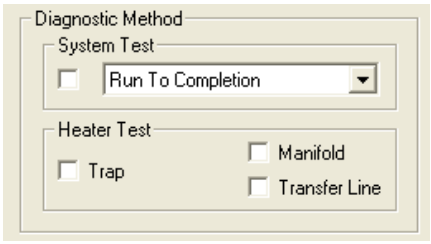
The Monitor and Event Message window detail the results.

```
13:59:35  Diagnostics: Started
13:59:35  System Test: Started
13:59:37    System Verification Results
13:59:37      Basic Hardware Test:      Passed
13:59:37      Vacuum Test:              Passed
13:59:37      RF Test:                  Passed
13:59:37      Waveform Test:            Passed
13:59:37      Acquisition Test:         Passed
13:59:37      Basic Heater Test:        Passed
13:59:37      Ionization Test:          Passed
13:59:38  System Test: Completed
13:59:38  Diagnostics: Completed
```

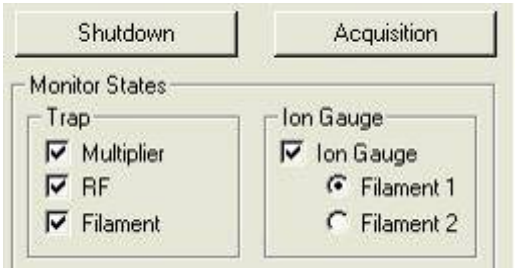
If a fault occurrs, the message indicates what test failed and the source of the problem.

```
14:04:27      Acquisition Test:         Passed
14:04:27      Basic Heater Test:        FAILED
14:04:27        THE FOLLOWING THERMOCOUPLES REPORT OPEN OR UNPLUGGED:  MANIFOLD.
14:04:27      Ionization Test:          Passed
14:04:27  Diagnostics:  FAILED.
14:04:27  System Test: Completed
14:04:27  Diagnostics: Completed
```

To perform a more detailed test of the heater zones, click the box of the zone to be tested. These tests can take up to 13.5 hours for the trap, 2 hours for the manifold, and three hours for the transfer line. The manifold and transfer line tests can be run simultaneously.

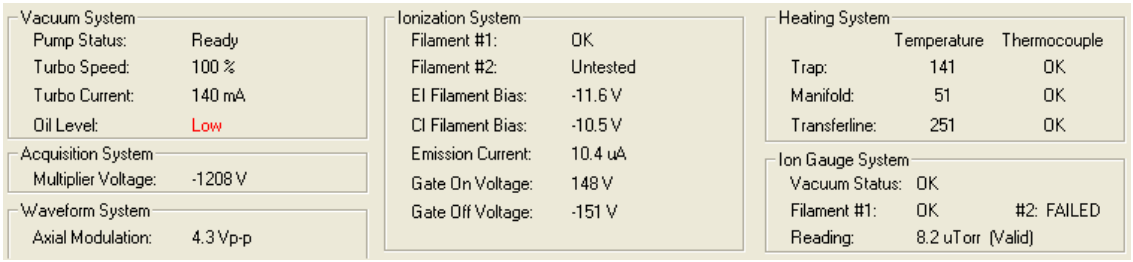


The far right has Monitor States, which monitor the multiplier, rf, Filament, and Ion Gauge if present. Click the check box to activate. Some elements of the diagnostic display are active when some trap components are off.



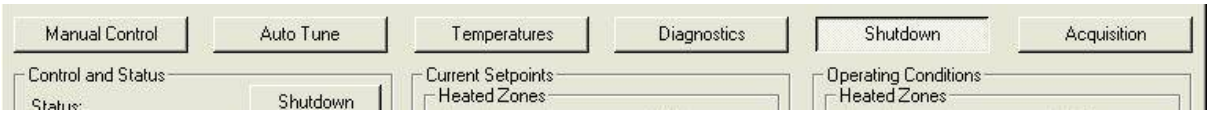
NOTE: The following is from a 225-MS. The 210-MS and the 220-MS do not have the Oil Level readback.

The temperature for each heated zones is displayed.



Shutdown

The shutdown procedure shuts the system down in an orderly fashion.



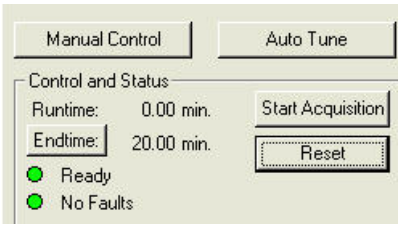
Click Shutdown to turn off the heaters and slowly turn the turbo pump turn off.

To restart the system after activating shutdown, click reset.

After the temperature zones are cool, turn the main power switch on the back panel Off. Manually vent the system for at least 5 minutes using the lever on front panel.

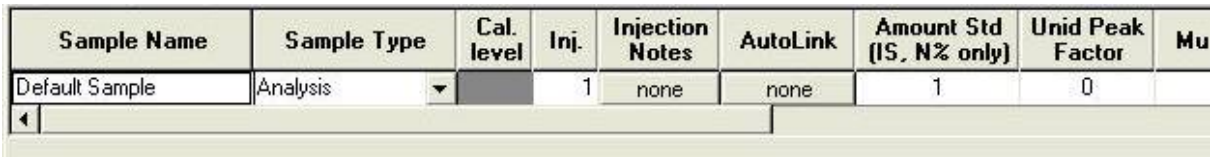
Acquisition

When Acquisition is first opened, it loads the information for the active method.



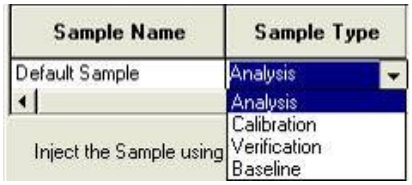
After a few moments the Ready red lights turn green to indicate that the MS is ready. If the GC and/or AutoSampler are ready there is a Not Ready message at the top of the screen. After the GC and AutoSampler come to a ready state, the not ready message changes to Ready. To determine the individual ready states of the components, go to the top pull down menu under Windows and see the states for the components.

An analysis can be run as a single sample or through an automated sequence. To run a single sample, go to the top Inject menu and Select inject single sample.

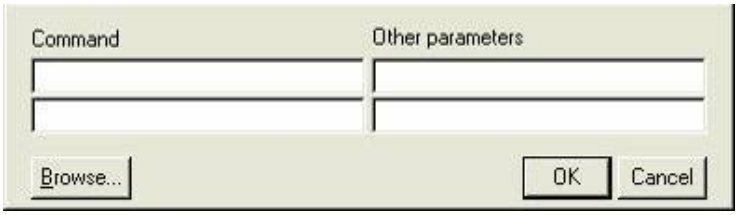


Thee fields in the Inject Single Sample dialog can be edited. Enter the correct information about sample name, vial position and injection volume if an AutoSampler is used, and data file path. After entering this, click the inject button. If an AutoSampler is not used, inject the sample the sample manually when the GC ready light is displayed on the GC keyboard.

Change the sample type by double-clicking.



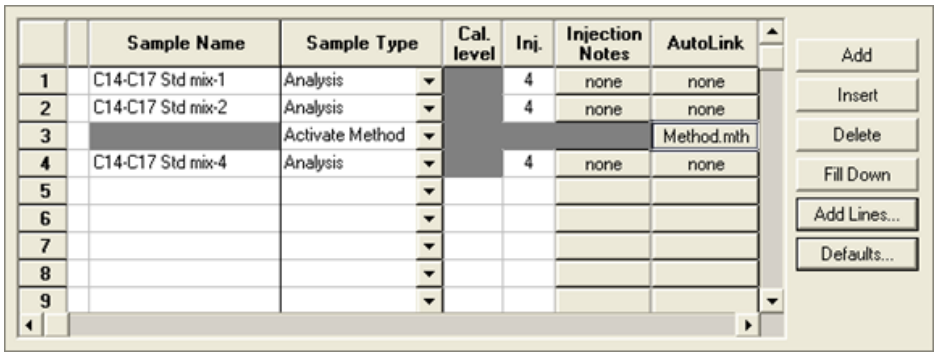
Perform the same procedure for injection notes. Notes are saved with the data file. AutoLink is similiar.



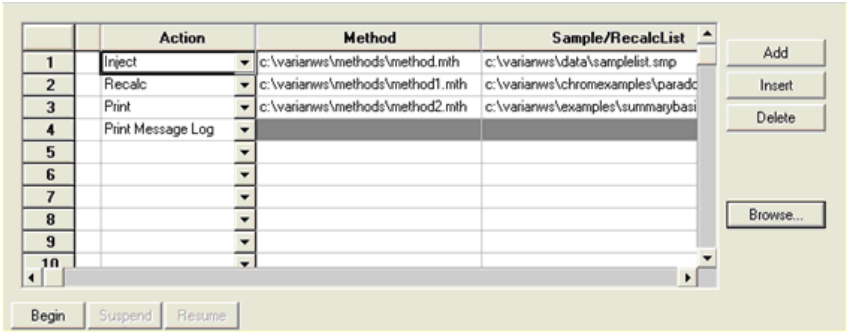
Enter a command to execute a program after data file acquisition is completed. This can be a program to activate a Custom MS Reports. Use the browse command to select the command file.

Use the RecalcList button to create a list of samples for data processing. This saves time creating the list.

To perform automated injections of a group of samples, build a sample list and then a sequence list. An example of a sample list follows. Activate this view from the pull down menu under File, New Sample List. The list must be created from an empty table.The entry fields are the same as the information in this section for single sample injections.



After creating a sample list, created a sequence. Select Inject for action, type the name of the method, and type the name of the sample list. Click Begin to start the sequence.



Configuring the Real-Time Chromatogram Display

During an analysis, observe the chromatogram in the System Control by selecting Chromatogram, Spectrum, or both.

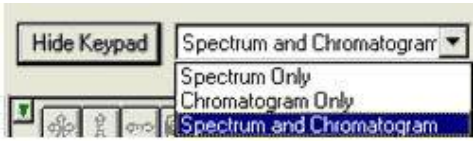
Choosing the Chromatogram only option displays a live chromatogram.

Click Hide Keypad to expand the chromatogram and hide the text information at the top.

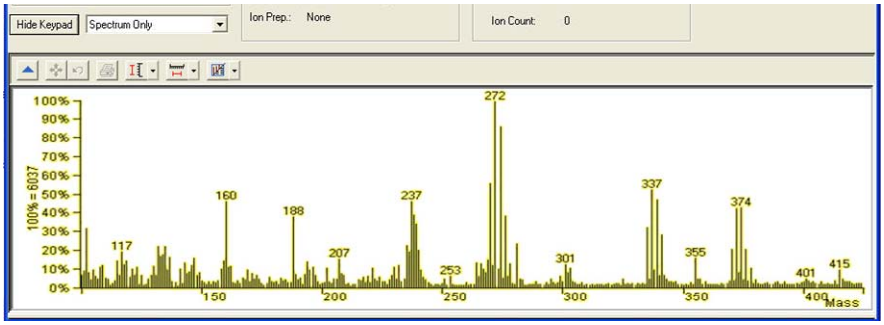
Configuring the Real-Time Spectrum Display

The spectrum can be observed during acquisition. Selecting the time selector mode in the chromatogram display stop the real-time update of the spectrum display.

Display the Chromatogram, Spectrum, or both.



Choose Spectrum Only to display a spectrum as it is acquired.



Parameters That Affect EI Operation

Electron Multiplier Gain

Normal MS operation assumes that the electron multiplier produces about 10^5 electrons per ion. This is accomplished automatically with Auto Tune.

The AGC software operates on information derived from the prescan measurement of the TIC (the AGC peak). (See “MS Method Scan Functions” on page 61 for details of scan function).

Unlike the ionization time or filament emission current that can alter the actual number of ions created in the ion trap, changing the electron multiplier gain only alters the amplification of the ion current signal of ions after they are scanned out of the ion trap. Thus, when the multiplier gain is changed, there is no change in the actual quantity of ions formed and measured in the prescan measurement, but the peak area of the AGC peak changes. The AGC software misinterprets this change in peak area as a real change in the number of ions created in the ion trap and adjusts the ionization time accordingly. An incorrect ionization time may cause a change in mass resolution. The AGC software is dependent on the multiplier gain remaining constant in order to measure the quantity of ions in the ion trap correctly and set the proper ionization time.

Under certain circumstances (low background, or small signal) increasing the electron multiplier gain by +100 or +200 volts above the 10^5 gain can decrease the detection limit. The same multiplier gain must be used for determining the calibration curve and analyzing unknown samples.

Axial Modulation

The number of ions stored in the ion trap is proportional to the ionization time and the filament emission current. Although the trap can store a maximum of about 10^6 to 10^7 ions, space-charge repulsion occurs when the number of ions exceeds 10^4 to 10^5. Space-charge interactions cause a loss in unit mass resolution. To overcome this limitation, a small ac voltage, the axial modulation voltage, is applied to the endcap electrodes.

The axial modulation voltage is applied at a fixed frequency and amplitude during the ramp of the rf voltage. The frequency of the axial modulation voltage is 485 kHz, which is about one-half of the frequency of the rf voltage. Only when an ion is about to be ejected from the ion trap cavity is it in resonance with this frequency. When an ion comes into resonance with this frequency, it moves away from the center of the trap, where the field generated by the rf voltage is zero (and space-charge effects are strong), into a region where the field produced by the rf voltage is strong (and space-charge effects are small). As a result, the ejection of the ion is facilitated, and mass resolution is significantly improved. The default axial modulation voltage is 4.0. Once the optimum axial modulate ion amplitude has been set for a given instrument, it need not be changed.

Emission Current

The number of ions formed in the trap is a function of both the ionization time and the intensity of the electron beam. In general, increasing the filament emission current increases the quantity of ions produced. The relationship between the filament emission current and the measured TIC, which is the number of ions generated in the ion trap, is not strictly linear. In particular, the emission current and the measured TIC do not vary linearly for emission current values above 40 µA and at high sample concentration.

Using a high emission current can increase the sensitivity. In EI/MS/MS, the MS/MS isolation step eliminates the higher background that would normally arise from a high emission current.

Ion Trap Temperature

After the system is shut down and the ion trap vented, use an initial trap temperature of 220°C to rapidily remove water vapor. After this, reduce the trap temperature to 150-175°C to extend the turbomolecular vacuum pump lifetime. Some applications may require higher temperatures. In general use the lowest temperature which provides acceptable chromatography. Bakeout can be done overnight and the temperature reset to operating conditions.

The trap temperature must be high enough not to affect chromatographic performance Use a trap temperatures between 50 to 75°C below the ending temperature for the GC column temperature ramp, without compromising chromatographic performance.

Certain compounds, such as straight chain hydrocarbons, fragment more at hotter ion trap temperatures.

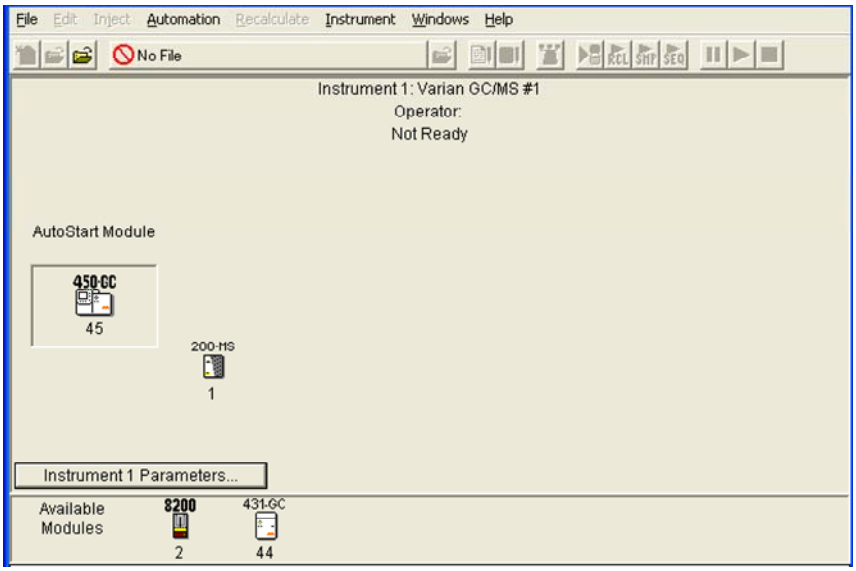
AGC Target TIC Value

In EI mode with AGC on, the target TIC value determines how many ions AGC allows into the ion trap during the calculated ionization time. While increasing the target TIC value increases peak heights, increasing it too far results in a loss of mass resolution. This is observed as mass misassignments and/or incorrect isotope abundance ratios. For full-scan EI operation, a target TIC of 20,000 is a good starting point. Under special circumstances, e.g., MS/MS, a much lower target TIC is required. As the m/z distribution of the stored ions becomes smaller, fewer ions can be trapped without a loss of resolution.

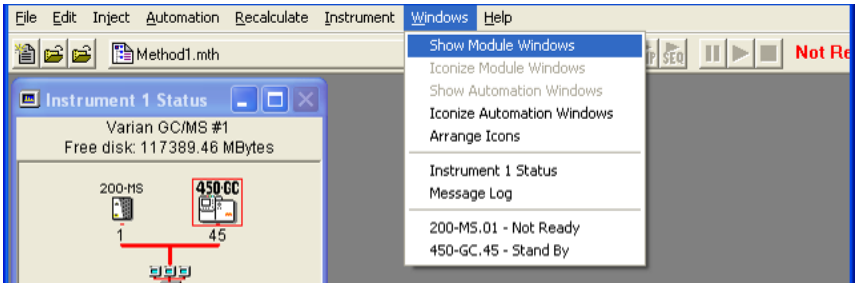
Controlling the 450-GC

450-GC Instrument Window

After configuring the 450-GC in MS Workstation, view the Instrument Window to monitor the status of all modules assigned to the instrument, to perform injections of one or more samples, and to perform batch recalculations.



Double-click in this area or select the instrument from the Instrument menu to view the 450-GC Status and Control window.

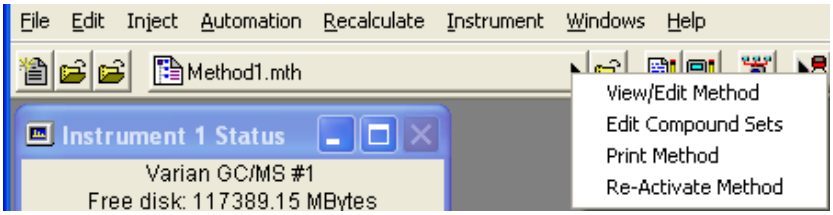


If the Status and Control Windows for the configured modules are not displayed, select **Show Module Windows** from the Windows menu.

Elements of System Control Toolbar

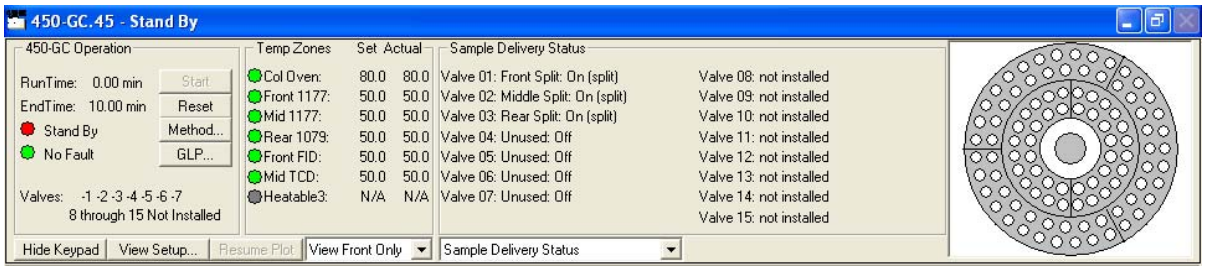
The System Control Toolbar has tools for common tasks. Rest the cursor on a button to display a short description. The buttons that control the SampleList, Sequence and RecalcList are available after a corresponding automation file is activated.

Click the Active Method button for additional options.



450-GC Status and Control Window

Initially the 450-GC Module Window is similar to the following. The window shows the 450-GC Operation parameters: RunTime, EndTime, Method State, and Fault State. The Start, Reset, and Method buttons control the 450-GC.

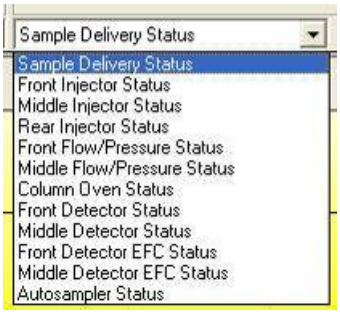


Use the 450-GC Window to display the 450-GC Setup dialog, to select the detector to view, and to select the component status to view.

Select the detector signals to view in the real time chromatogram from the menu.

View multiple detectors horizontally or vertically.

Change the component status display to view the status of each GC component.



Click a temperature entry to view a detailed component status.

Access the 450-GC Setup dialog from View Setup.

The installed hardware is listed. Change the set up from the 450-GC front panel or from MS Workstation.

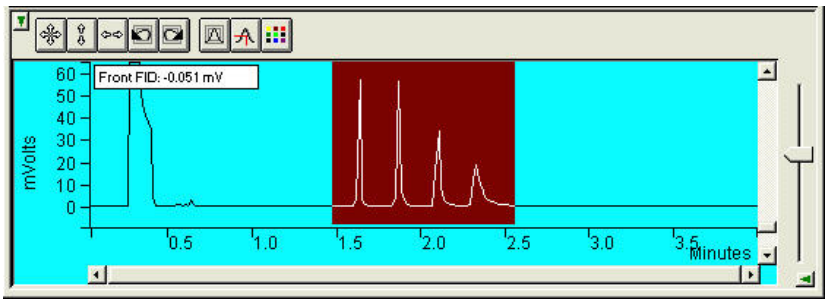
The detectors installed on the 450-GC, display their signals in real time. The configuration of the chromatogram is the same for all.

The 450-GC Module Window can show the chromatogram display or continue to show the signal after the run.

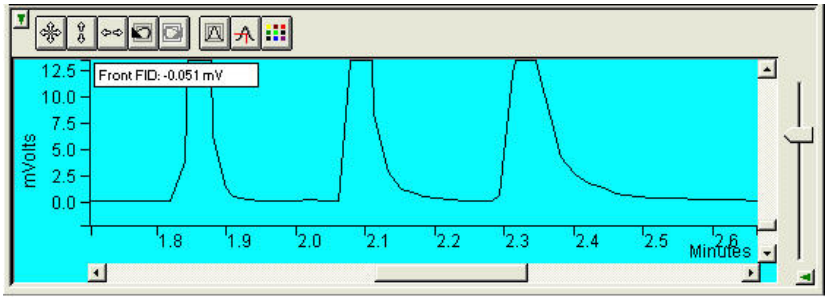
In the chromatogram area of the 450-GC Window the following can be performed:

- Hide/unhide the Toolbar.
- Set both the amplitude and time axes to full scale.
- Set the amplitude axis to full scale.
- Set the time axis to full scale.
- Use these buttons to move between stored scalings.
- Enable/disable the Auto Scale feature.
- Enable/disable the cursor display.
- Select the background color for the display.

Drag an area of the display to view a more detailed section of the plot, or zoom in both axes by pressing and holding the left mouse button on the spot you wish to enlarge. (Hold the Shift key down to zoom out.)



Adjust zero offset. Adjust amplitude scale.

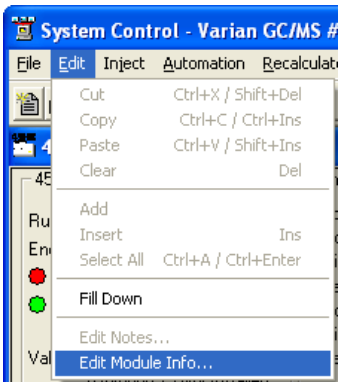


Adjust time scale.

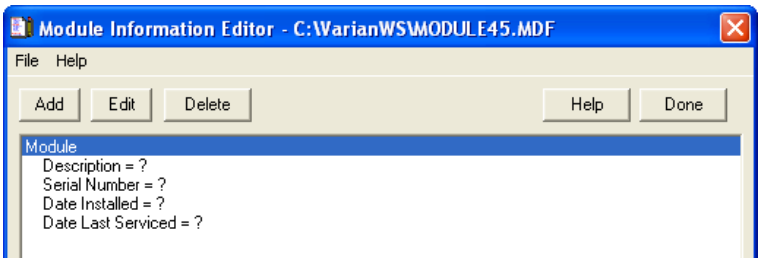
Hide/unhide vertical amplitude scale slider.

Documenting Module Information

Use the Module Information Editor from the Edit menu to document the configuration of your modules, their installation, and most recent service dates, and other information.



Click the module window to ensure it is active, and then click Edit Module Info.



Add and edit sections and items in sections.

The injections value is updated each time an injection is performed.

Select Help for details on creating and editing module information.

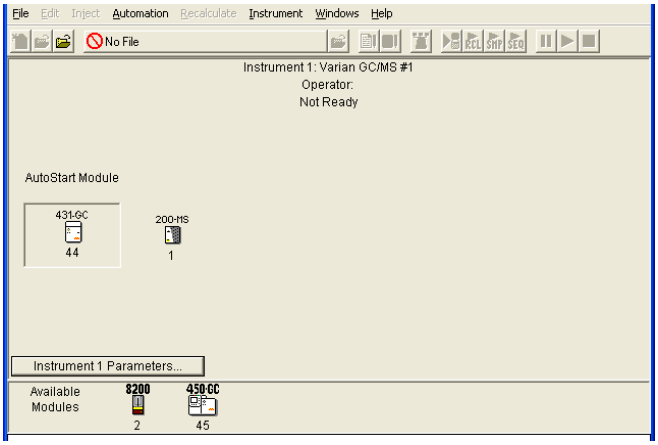
Click Done to close the window.

Module information is copied into Data Files that are generated after the injections are done and can be included in the Run Log portion of the results report.

Controlling the 431-GC

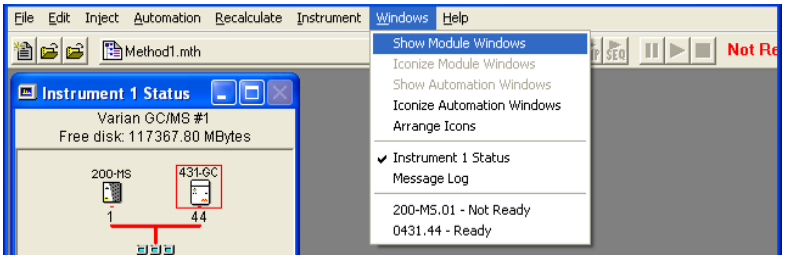
431-GC Instrument Window

Use the Instrument window to monitor the status of all modules assigned to the instrument, perform injections, and perform batch recalculations.



Double-click the background of the Instrument window or select the instrument from the Windows menu to view the 431-GC Status and Control window.

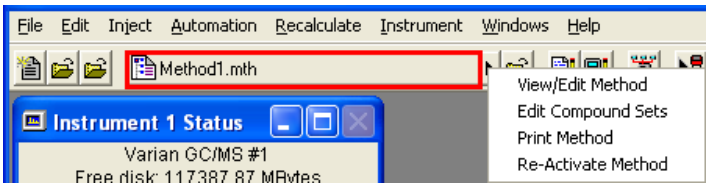
If the Status and Control Windows for the modules configured in the instrument are not displayed, select Show Module Windows from the Windows menu.



System Control Toolbar

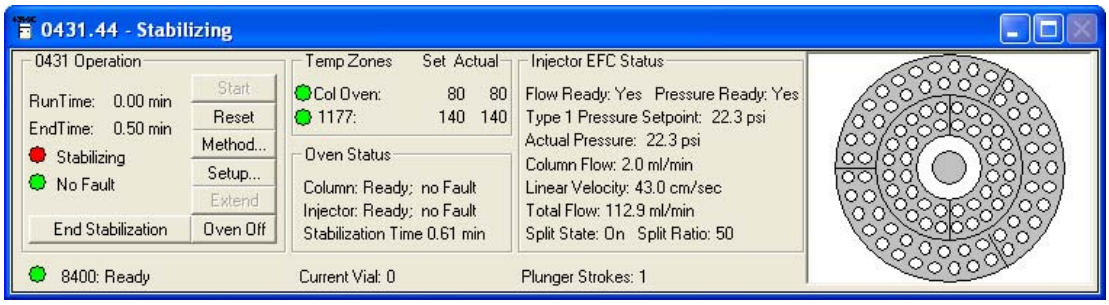
The System Control Toolbar provides for common tasks. Rest the cursor on a button to display a short description. The buttons controlling the SampleList, Sequence and RecalcList are available after an automation file is activated.

Click the Active Method button to show additional options.

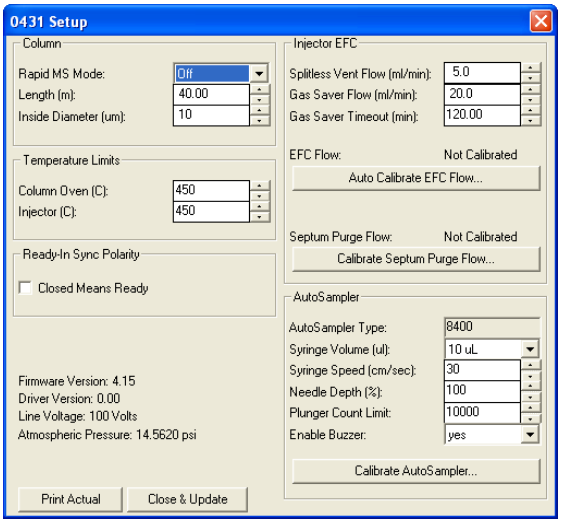


431-GC Status and Control Window

The left side of the 431-GC Module Window shows the 431-GC Operation parameters: RunTime, EndTime, Method State, and Fault State. The Start, Reset, and Method buttons control the 431-GC. The middle area shows the status of the heated zones and EFC. The right side shows the AutoSampler rack, if present.

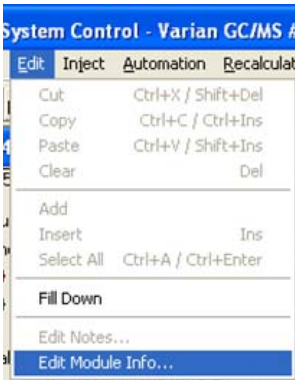


Access the 431-GC Setup dialog from Setup , which lists the installed hardware.

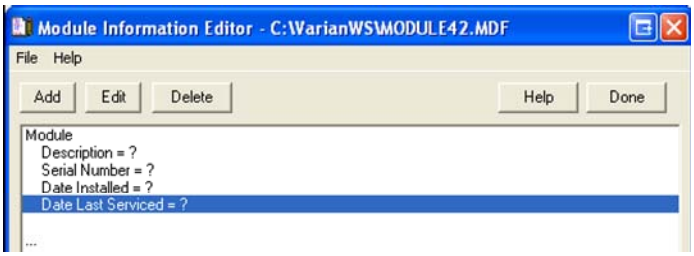


Documenting Module Information

Document the configuration of your modules, their installation and most recent service dates, and other information using the Module Information Editor. Select Edit Module Info from the Edit menu.



Click the module window to ensure it is the active window, and then click Edit Module Info. The Module Information Editor window opens.



Add, edit, or delete entries by double-clicking a parameter such as Description or Date installed.

Click **...** to create a new section.

The injections value is updated each time an injection is performed.

Module information is added to the Data Files and can be included in the Run Log section of the results report.

MS Method Scan Functions

Introduction

The MS analyzes ions as their mass-to-charge (m/z) ratios and relative abundances in the spectra. The mass spectrum is represents the ion intensities versus the mass-to-charge ratio.

The MS creates the mass spectrum with an ion-trap analyzer. This type of analyzer differs from beam transport analyzers such as magnetic sectors, quadrupoles, and time-of-flight instruments where the ions to be separated pass through a sequence of fixed electromagnetic fields. Instead, the ion trap confines the ions within a single region where they experience time-dependent electromagnetic fields.

Sample analysis with an ion trap analyzer is divided into several steps:

Sample Introduction: Compounds are introduced from the transfer line to the ion trap analyzer through the direct coupled capillary column.

Sample Ionization: The compound is ionized in the mass spectrometer by either:

- destabilizing its molecular structure, causing an electron to be removed from somewhere on the molecule (Electron Impact/Ionization) (EI).
- pressuring the MS with a selected reagent gas; e.g., methane, performing EI on the gas to form reagent ions, and allowing ion-molecule reactions to occur between the compound and the reagent ion (Chemical Ionization) (CI).

Sample Fragmentation: Depending on the original structure and the excess destabilizing internal energy, the ionized compound (molecular ion) fragments. This process forms fragment ions and neutral fragments.

Ion Storage: The ions are stored and stabilized in the trap and travel in defined orbits. Helium buffer gas helps to focus the ions into more compact orbits which produce sharp peaks. Helium is used because it does not ionize as readily as the analyte molecules. While helium ions are the most dominant species in the trap, they are not stored, but are pumped away as soon as they are formed.

Ion Analysis: A radio frequency (rf) (1.1 MHz) voltage is applied to the ring electrode encircling the trap cavity. As the voltage increases on the ring electrode, ions are sequentially ejected from the trap according to their mass-to-charge ratio. A small ac voltage (axial modulation voltage) of fixed frequency and amplitude is also applied to the endcap electrodes during the analysis to improve ion injection and unit mass resolution.

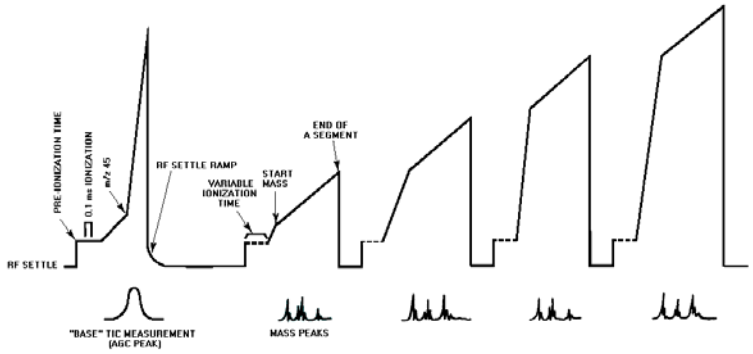
Ions are created by electron ionization or chemical ionization. A scan function represents the sequence of ion trap operation. It shows the variations in time of the rf potential applied between the ring electrode and the end cap electrodes, and any supplementary waveforms applied to the cap electrodes.

MS Method Electron Ionization

EI with AGC

The ion trap has a maximum storage capacity, beyond which mass resolution and spectral quality deteriorate. More ions are produced with longer ionization times. Automatic Gain Control (AGC) controls the ionization time to keep the number of ions in the trap at the optimum level.

The AGC scan function has a prescan and up to six scan segments. The prescan uses resonance ion ejection. The number of ions detected in the prescan is used to calculate the ionization time for the six scan segments. The following figure illustrates four scan segments correspond to the following four portions of the mass range (default values): 10 to 99 m/z, 100 to 249 m/z, 250 to 399 m/z, and 400 to 650 m/z. One scan involves one complete ramping of the rf voltage over the mass range selected by the user. The rf voltage is ramped at a constant rate of approximately 5600 m/z per sec. One complete scan at this fixed rate produces a microscan.



The AGC Scan Function

The AGC software automatically selects an ionization time from 10 µsec to 65 msec for each of the six scan segments of the microscan, depending on the amount of analyte in the ion trap and the tuning parameters. An estimate of the number of ions formed in the ion trap is provided by a short prescan that consists of a 0.1 millisecond ionization period. For low levels (e.g., for baseline or small GC peaks) the maximum ionization time of 65 milliseconds is selected, which offers maximum sensitivity. As the amount of analyte increases, the ionization time decreases automatically to prevent saturating the ion trap.

The ion signals in each microscan are scaled automatically to correct for the variation in ionization time. Microscans are averaged to improve the spectral quality.

Ion Formation

In the EI mode, electrons are passed through the ion trap cavity during the ionization period. They collide with the neutral sample molecules present and transfer some of their energy to the molecules. These energetic molecules decompose through a series of reactions producing ions and neutral fragments. The fragment ions make up the mass spectrum. The degree of fragmentation is a function of the internal energy of the molecules, which is a function of the energy imparted by the electrons, as well as the ion trap temperature and the axial modulation voltage amplitude.

The ionization time is the time (between 10 µs and 65 milliseconds) during which the electron gate voltage is positive, and the electron beam from the filament is enters the ion trap. The electron beam generates ions by colliding with sample and/or background molecules which are present within the ion trap. The AGC software provides control of the ionization time so that the quantity of ions can be maintained at the optimum level.

The number of ions formed in the trap is also a function of the intensity of the electron beam. In general, increasing the filament emission current increases the quantity of ions produced. The relationship between the filament emission current and the measured TIC (i.e., the number of ions generated in the ion trap) is not a strictly linear one. In particular, the emission current and the measured TIC do not vary linearly for emission current values above 40 µA and at high sample concentration.

Both the ionization time and the intensity of the electron beam control the number of ions formed, and that the ion trap performs best (producing the highest quality spectra with good resolution) when an optimum quantity of ions (or “charge”) exists.

AGC Prescan

The 0.1 millisecond ionization is followed by the ramping of the rf voltage to eject the permanent background from 35 m/z to an upper mass limit selected by the user. This upper mass limit is defined as the background mass. The default value for the upper mass limit is 45 m/z; as a result, all masses below the background mass (i.e., those masses corresponding to the chemical background) are ejected from the trap.

The rf voltage is then ramped to its maximum value, and all ions with masses above the background mass are ejected from the ion trap and are detected by the electron multiplier. The electron multiplier produces a signal proportional to the number of ions detected.

The ion current measured during the AGC prescan is the AGC peak area. The AGC peak area is proportional to the number of ions formed during the prescan ionization. The AGC software uses the measured ion current as a reference to optimize the ionization time for each scan as a function of analyte concentration.

Scan Segment Setup

The prescan is followed by the first segment of the six scan segments. Each segment has two parts: a setup period and a scanning period. Each setup period has the following four stages:

- First stage: The rf voltage is set to near 0V for 2 milliseconds. The rf voltage generator circuit stabilies while clearing the trap cavity of all ions.
- Second stage: The rf voltage is set to, and stabilizes at, the storage voltage, selected or trap all ions of interest.
- Third stage: The electron gate is turned ON. Energetic electrons from the heated filament are accelerated into the ion trap, interact with sample molecules, and form sample ions. After ionization, the electron gate is turned OFF. The newly formed ions stabilize in their orbits at the storage voltage. This stabilization period is the cool time. The length of this period is fixed.
- Fourth stage: The electron multiplier is made ready, and the rf voltage is ramped quickly from the storage voltage to the value need to scan masses.

Mass Scanning

During mass analysis, the rf voltage is ramped from a low voltage to a higher voltage.

The ion trap operates in the resonance ejection mode. In this mode, at low rf voltage (for example, at the storage voltage) most ions have stable oscillations in the ion trap cavity. However, as the rf voltage is increased, ions of progressively greater mass-to-charge ratios become unstable and are ejected from the cavity.

The voltage at which an ion is ejected from the ion trap cavity is the resonance voltage. At a voltage below the resonance voltage, an ion travels in a stable orbit, oscillating along all three axes. At or above its resonance voltage, the trajectory of the ion becomes unstable. As the rf voltage increases above the resonance voltage, the amplitude of the oscillation of the ion increases most rapidly in the axial direction. As a result, when ions are no longer stable in the ion trap cavity, they are ejected from the cavity in a tightly collimated beam upward and downward. The ejection of ions of each mass-to-charge ratio occurs over a very short time period. One half of the ions go up; these ions strike the top endcap and are neutralized. The other half of the ions go down and pass through the holes in the bottom endcap. Many of these ions strike the electron multiplier and are detected.

The rf voltage is ramped at a constant rate of about 5600 m/z per sec. One complete scan at this rate produces a microscan. Depending upon the mass range and scan time, more than one microscan may be obtained during each scan. (The number of microscans per scan for each set of mass range / scan time conditions selected is displayed on the data system monitor.) If two or more microscans are obtained, they are averaged by the SAP Board and then stored as one mass spectrum. Averaging the microscans improves spectral quality.

At the end of the scanning period, the rf voltage is again set to near 0V, and the electron multiplier is put into STANDBY. The entire process (setup and scanning) is repeated up to six times per microscan, once for each of the six segments.

Basic Equation AGC

The AGC software sets the ionization time to maintain the optimum quantity of ions for each of the segments according to the following equation:

$$IT_a = IT_p \times \frac{TIC_t}{TIC_m} \times SF_a$$

where:

IT_a is the ionization time for segment “a” in a six segment microscan;

IT_p is the ionization time of the prescan (default value of 0.1 millisecond);

TIC_m is the area in counts of the total ion AGC peak from the prescan;

TIC_t is the tunable target TIC value used as a reference for the prescan measurement calculations; and

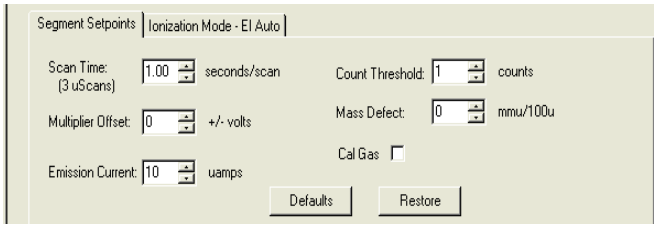
SF_a is the scale factor for segment “a”. It is a percentage of the actual ionization time (IT_a) that permits individual adjustment of the response and resolution of each segment.

Increasing the target TIC increases the ionization time for all the segments; decreasing decreases the ionization time. The target TIC is a general resolution adjustment for the entire mass range (all six segments together).

It is apparent that when the TIC increases because the ion trap is generating more ions (usually due to an increase in sample or background pressure), then the AGC software reduces the ionization time automatically, and vice versa. Also, if the target TIC is increased, the ionization time for any given pressure increases and the ion trap creates more ions. Likewise, reducing the target TIC value decreases the number of ions in the trap.

Software Parameters

Segment Setpoints



Scan Time

Set the scan time from 0.100 to 5.000 seconds per scan. Below the scan time is the number of microscans per scan for the selected mass range and scan time. The number of microscans per scan is computed automatically. It is displayed for information only. The minimum duration for the scan time is determined by the selected mass range.

Multiplier Offset

To improve detection limits, increase or decrease the multiplier voltage by 300 volts of the Electron Multiplier 10^5 gain. The same multiplier gain must be used for determining the calibration curve and analyzing unknown samples.

Emission Current

The number of ions formed is a function of the ionization time and the intensity of the electron beam. In general, increasing the filament emission current increases the quantity of ions produced. The relationship between the filament emission current and the measured TIC (i.e., the number of ions generated in the ion trap) is not strictly linear. In particular, the emission current and the measured TIC do not vary linearly for emission current values above 40 µA and at high sample concentration.

In certain cases, using a high emission current can increase the sensitivity. For example, in EI/MS/MS the MS/MS isolation step eliminates the higher background that normally arises from a high emission current. Set the emission current from 5 to 100 µA.

Count Threshold

The minimum number of counts per sampling interval before a signal is recorded. (The maximum number of counts per sampling interval is 4095.) Set the peak threshold to a value from 0 to 1000 counts; it is typically set to 0 or 1.

Mass Defect

Mass defect is the difference between the nominal mass of an atom (or ion) and its exact mass. The MS reports molecular weights to the nearest integer mass unit. The software determines the mass. If the exact mass of an ion is close to the dividing line between integer masses, it may be assigned to the wrong mass. This is more likely for molecules with higher molecular weights, since the mass defects for several atoms may add together to produce a sizable mass defect. The mass defect parameter may be set from -300 mu per 100u to +300 mu per 100u. The formula for calculating the mass defect parameter is:

$$MassDefect = \frac{ActualMass - IntegerMass}{IntegerMass} x10^5 mu/100u$$

For example, hexachlorobenzene (C_6Cl_6) with an exact mass (base peak) of:

$$(6x12.0000)+(5x34.9689+(1x36.9659)=283.8104$$

has a mass defect of:

$$(283.8104-284)/284x10^5=-66.76mu/100u$$

Similarly, dodecane ($C_{12}H_{26}$) has an exact mass of:

$$(12x12.0000)+(26x1.0078)=170.2028$$

and a mass defect of:

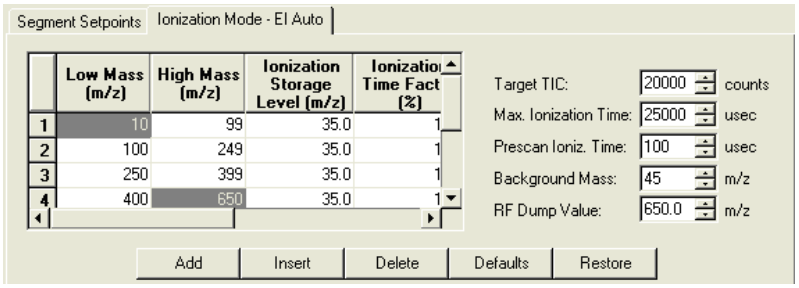
$$(170.2028-170)/170x10^5+119.29mu/100u$$

Obviously, if a sample contains both compounds, the mass defect parameter cannot be optimized in a single segment. For most analyses set the mass defect to 0 to avoid mass misassignments, or program it with multiple segments.

Cal Gas

Turn the calibration gas on during an acquisition by clicking the Cal Gas checkbox.

Ionization Mode - EI Auto



Mass Range Segment Breaks

Each EI scan has four mass segments: 10 to 99 m/z, 100 to 249 m/z, 250 to 399 m/z and 400 to 650 m/z. For certain applications, the mass segments can be adjusted. Click Insert to Add additional segments (maximum of 6 segments).

Ionization Storage Level

Each segment has its own ionization storage level. This corresponds to the rf voltage used to hold ions in the trap during the ionization period. It affects ion storage in two ways— the storage efficiency of higher mass ions increases as the level increases, while lower mass ions are not stored if their mass falls below the cutoff. With AGC on, the default storage level is set to 35 m/z and all ions above 35 m/z are stored. This value gives good storage efficiency for ions up to 650 m/z, while not storing the 18 and 19 m/z ions from water vapor.

For certain analyses, increase the storage voltage to prevent the storage of ions produced from the solvent. For example, to exclude ions produced from methanol (mass 32 and below), set the storage voltage to 38 m/z for all segments. Keep the EI background mass greater than or equal to the segment ionization storage voltage.

Ionization Time Factor

The Ionization Time Factor is a secondary factor that determines how well the MS is tuned. The Ionization Time Factor, a percent, is multiplied by the calculated ionization time (determined by the AGC pre-scan pulse) to give the actual ionization time. The default value is 100%. The Ionization Time Factor determines the actual ionization time for each segment; thus, it determines the number of ions in the ion trap for that segment

The calculated ionization time, determined by the AGC pre-scan pulse, is generally the optimum value for segment 2. At lower masses (segment 1),, an actual ionization time of as low as 75% (never lower than 50%) of the calculated ionization time may provide a better tune. And for higher masses (segments 3

and 4), an actual ionization time of up to 125% (and never higher than 200%) of the calculated value may provide better results.

As the ionization time factor is increased (actual ionization time increased), the peak height increases. However, the resolution of adjacent mass peaks may decrease and the peak shape might distort.

Target TIC Value

In EI mode with AGC on, the target TIC value determines how many ions AGC allows into the ion trap during the calculated ionization time. While increasing the target TIC value increases peak heights, increasing it too much results in a loss of mass resolution. This would be mass misassignments and/or incorrect isotope abundance ratios. For full-scan EI operation, a target TIC of 20,000 is a good starting point. Under special circumstances, e.g., MS/MS, a much lower target TIC is required. As the m/z distribution of the stored ions becomes smaller, fewer ions can be trapped without a loss of resolution.

Maximum Ionization Time

Sets the limit for the longest ionization time for AGC. For maximum sensitivity, start with the default value of 25,000 µsec. In certain cases a smaller value may be used, e.g., to reduce unwanted ion-molecule reactions. The highest Maximum Ionization Time is 65,000 µsec.

Prescan Ionization Time (µsec)

Determines the number of ions formed for the prescan. This value is used to calculate the ionization time for the analytical scan. The preset value of 100 µsec works for EI operation. If few ions might be formed in the prescan (e.g., EI-MS/MS) use a large value such as 1500 µsec. Be careful when using a large value because so many ions may be made in the EI mode that the prescan becomes saturated and AGC no longer functions properly.

Background Mass

The lowest mass used to determine the target TIC (total ion current) value. All ions of lower mass are ejected from the ion trap before the AGC prescan pulse. Set the background mass from 10 m/z to 300 m/z; it is typically set to 45 m/z. The background mass should always be set at least two m/z higher than the Ionization Storage Level.

rf Dump Value (m/z)

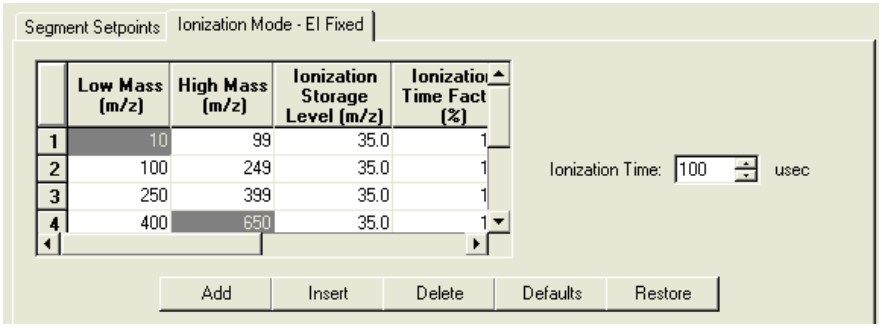
The high m/z for the prescan. It should always be as high or higher than the analytical scan range high mass. In most cases, use the default value of m/z=650. In certain cases, operating at 400 or 450 (matching the analytical scan) may allow operation in spite of high mass noise.

Ionization Mode - EI Fixed

When AGC is off, a fixed ionization time scan function coordinates the processes that occur in the ion trap. This scan function, has four segments that compare qualitatively to those the Auto scan. It may contain up to six segments. However, the fixed ionization time scan function has no prescan. Thus, the ionization times

for each segment do not vary as a function of sample concentration. Set the Ionization Time from 10 to 65,000 µsec.

Manual tuning in Fixed mode is performed by altering the Ionization Storage Levels and Ionization Times for each segment of the microscan.



MS Method Chemical Ionization

Introduction

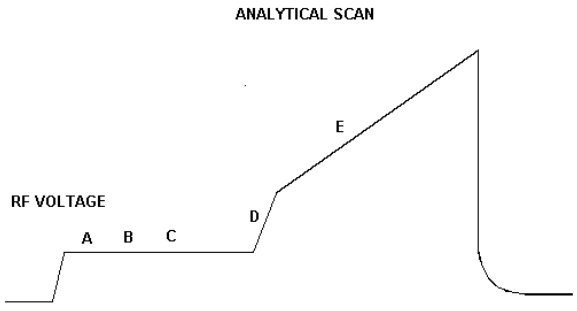
Chemical ionization (CI) provides mass spectral data that complements electron ionization (EI) data for the analysis of complex compounds. In the CI mode of operation, a CI reagent gas is introduced into the ion trap analyzer. The reagent gas is ionized by EI. Then, the sample molecules are ionized by ion molecule reactions with the reagent gas ions.

CI is a softer ionization technique than EI. That is, CI imparts less energy to the sample molecules than EI. The ionized sample molecule fragment less, and an ion indicative of the molecular weight may be seen. CI mass spectra often provide structural information not be available from EI mass spectra.

CI Scan Function

EI space charge control uses the integrated ion current from a fixed ion time prescan to calculate the analytical scan ionization time. In contrast, CI space charge control does not use a fixed ionization time prescan to measure the charge formed. CI uses a portion of the ions detected during the previous analytical scan to calculate the ionization and reaction times for the next analytical scan.

The following is a graph of the scan function.



A	Reagent gas ionization, time determined by the previous scan
B	Ejection of unwanted ions (i.e., non-reagent ions) using a CI ejection waveform
C	Reaction of reagent gas ions with sample molecules, time determined from previous scan

D Ejection of ions with masses lower than that of the background mass

E Acquisition of CI mass spectrum

Chemical ionization occurs by forming reagent ions by electron ionization. The reagent ions react with the sample to form product ions by ion molecule reactions. The ionization and reaction storage rf are maintained at the same level. Unwanted sample ions formed during the ionization of the reagent ions are ejected using a low frequency waveform before to the chemical ionization step.

The ion trap operates in a pulsed mode. The supply of reagent ions is created during the ionization pulse and consumed during the reaction period to form analyte ions. The number of analyte ions depends on the concentration of the analyte, the initial reagent ion intensity, and the reaction time.

Because the spectral intensity is proportional to sample concentration and reaction time, linear calibration curves can be obtained.

During the analytical scan, the following occur:

- The reagent gas is ionized for the time period determined by the previous scan.(A)
- All ions with a mass greater than the reagent ions are ejected, i.e., all EI ions from the sample. (B)
- Reagent gas ions react with sample molecules to form sample ions. (The reaction time was determined by the previous scan.) (C)
- Reagent gas ions are ejected. (D)
- The CI mass spectrum is acquired for the sample ions. (E)

All ions above a cutoff mass are ejected by applying a waveform between the ionization and reaction periods. This is perferred, since it eliminates all EI artifact ions. It should be noted that fragmentation can be observed in CI spectra due to energy imparted when the proton is transferred from the reagent ion to the sample molecule.

CI Ion Formation

In CI, ionization of sample molecules is a two-step process.

In the first step, reagent gas ions are formed as the reagent gas is ionized by interaction with electrons emitted by the filament.

In the second step, the reagent gas ions react with sample molecules in the ion trap to form sample ions. The four principal reactions between reagent gas ions and sample molecules are:

(A) Proton transfer: $(RH)^+ + M \rightarrow (MH)^+ + R$

(B) Hydride abstraction: $R^+ + M \rightarrow [M\text{-}H]^+ + RH$

(C) Association: $R^+ + M \rightarrow (MR)^+$

(D) Charge transfer: $R^+ + M \rightarrow M^+ + R$

where R^+ is the secondary reagent gas ion and M is the neutral sample molecule.

For methane CI, proton transfer (A) is the major reaction, and hydride abstraction (B) is the next most often observed reaction. For both, the resulting even-

electron ions are often relatively stable, and the observation of strong (M+1) or (M-1) ions is possible even if the EI spectrum of the same component shows no molecular ion. The exothermicity of the reactions determines the amount of energy; therefore, control the degree of fragmentation by selecting a suitable CI reagent gas. The proton affinities of some common reagent gases, known as proton transfer agents or Bronsted acids, range from 130 kcal/mol to 200 kcal/mol in the following order: methane, water, isobutane, and ammonia (with ammonia resulting in the "softest" ionization). Choose a suitable reagent gas, to obtain high specificity (i.e., less efficient detection of background or matrix interferences compared to the analyte) and molecular weight information.

The association or clustering reactions (C) typically have very low reaction rates, and the reaction products require rapid collisional stabilization. They are typically seen at much lower abundance then the (M+1) ion, but when (M+28) and (M+41) ions are observed using methane, they are useful for verifying the molecular weight.

The charge transfer reaction (D) produces a radical molecular ion (i.e., an ion with an odd number of electrons) that dissociates quickly, giving EI-like spectra. However, the energy deposited in the molecular ion and the resulting fragmentation pattern does not depend on the electron energy of the ionizing electrons. Common charge-transfer reagent gases are nitrogen and argon.

NOTE: Reagent ion formation can be complex. For example, for proton transfer CI with methane as the reagent gas, the gas ions are formed as follows:

First, methane is ionized to form two primary ions:

$CH_4 + e^- \rightarrow (CH_4 \bullet)^+ + 2\ e^-$

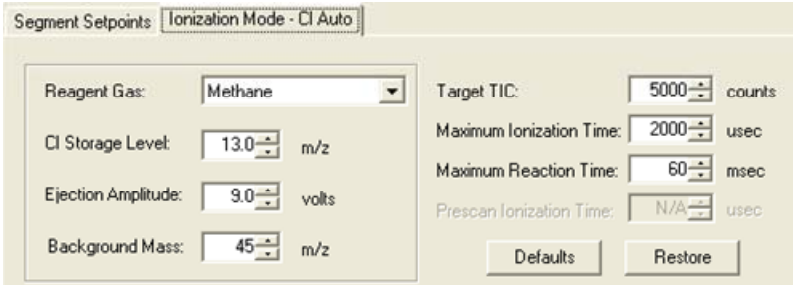
$CH_4 + e^- \rightarrow CH_3^+ + e^- + H^-$

These primary ions react very rapidly to form the secondary ions, CH_5^+ and $C_2H_5^+$:

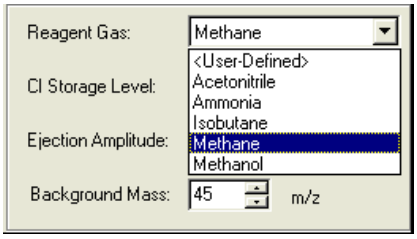
$(CH_4 \bullet)^+ + CH_4 \rightarrow CH_5^+ + CH_3 \bullet$

$CH_3^+ + CH_4 \rightarrow C_2H_5^+ + H_2$

CI Parameters



Reagent Gas



When a standard reagent gas is selected, default CI parameters are set automatically. You can optimize, parameters; Max. Ion Time, Max. React Time, CI Storage Level Ejection Amplitude (v), and Background Mass for sensitivity.

If you do change a CI parameter and set it incorrectly, you may not be able to operate properly in CI.

CI Storage Level

CI Storage level is the value of the smallest mass stored in the ion trap during the ionization of the reagent gas and the lowest mass stored during the reaction period. The CI storage Level is typically set lower than the mass of the reagent ion. Set the CI Storage Level from 5 to 150 m/z. The optimum CI storage level depends the on the molecular. Generally, use higher CI storage levels for higher molecular ions, without raising the storage level to cause ejection of CI reagent ions. For example, the molecular ion of the analyte is 352 m/z. Using acetonitrile, raising the rf storage level to 25 m/z may give better sensitivity than the default of 19 m/z. If the CI storage level is raised, the Ejection amplitude must be increased. For acetonitrile, raising the rf storage level from 19 to 25 m/z, requires an increase in the ejection amplitude from 15 to 25 volts. These values are determined empirically.

Ejection Amplitude (v)

Ejection Amplitude (v) is the voltage corresponding to a low mass ejection cutoff that is slightly higher than the mass of the largest reagent ion produced by the selected reagent gas. This voltage actively ejects unwanted ions (i.e., not reagent ions) that are produced during ionization. All ions with masses equal to or greater than the level established by this voltage are ejected before the CI reaction. When this value is set to 0, active ejection is disabled; otherwise, increasing the voltage decreases the ejection cutoff mass. Generally, higher CI storage values require higher ejection voltages. The voltage should not be set so high as to eject CI reagent ions.

Background Mass

Background mass is is greater than or equal to the mass of the largest reagent ion produced by the reagent gas. All ions with masses less than this mass value are ejected from the ion trap after the reaction between the reagent ions and sample molecules. The background mass level can be set from 10 to 300 m/z. For methane, ammonia, and isobutane, the reagent ion ejection levels are 45, 45, and 65 m/z, respectively.

Target TIC Value

In CI Auto mode, the target TIC value determines how many ions are allowed in the ion trap. The maximum value is 30000.

Maximum Ionization Time

Th maximum time that electrons, emitted from the filament, interact with reagent gas molecules to form reagent ions. Set the maximum ionization time from 10 to 2500 usec. For methane, ammonia, and isobutane, the maximum ionization time is usually set to 2000 usec.

Maximum Reaction Time

Maximum reaction time is the maximum time that reagent gas ions react with sample molecules to form ions. Set the maximum reaction from 1 to 128 milliseconds. For methane, isobutane, and ammonia, the maximum reaction time is typically set to 60 milliseconds.

Prescan Ionization Time

Prescan Ionization Time is used in MS/MS applicationsand is set at 200 μsec.

Default CI Parameters for Reagent Gases

Reagent Gas	Methane	Isobutane	Ammonia
Maximum Ionization Time (usec)	2000	2000	2000
Maximum Reaction Time (msec)	60	60	60
CI Storage Level (m/z)	13	19	13
CI Background Mass (m/z)	45	65	40
Ejection Amplitude (v)	9.0	15	9

Using Non-Standard CI Reagent Gases

Gases other than methane, ammonia, or isobutane can be used. If using a non-standard CI reagent gas, select the Reagent Gas labeled "User Defined"**.** Then type the name of the gas and the values for the CI parameters.

NOTE: When installing a new supply of a non-standard reagent gas, you must adjust the reagent gas pressure. After the pressure is adjusted properly, check the pressure at least once every day.

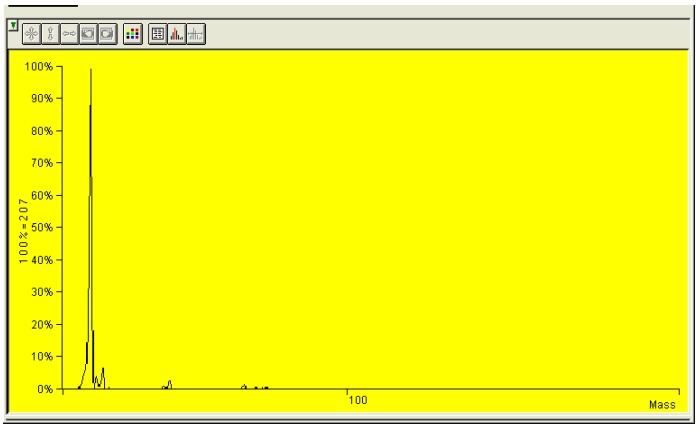
Optimizing the CI Background Mass

CI background mass eliminates reagent ions left after the reaction.

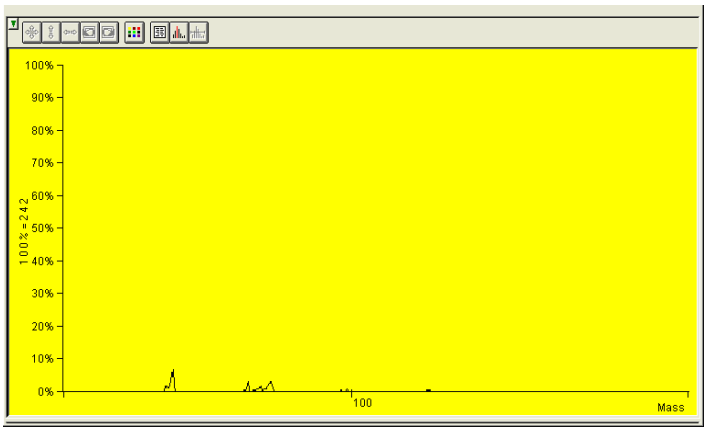
To optimize the CI Background Mass, do the following:

1. Connect the CI reagent gas.
2. Open the CI needle valve 6 to 7 turns counterclockwise.
3. Click the CI Gas control on the System Control.

4. Turn on the trap and observe the spectrum over the scan range in the acquisition method (do not use adjust CI Gas). Look for ions at the low end of the range. The following figure shows an acetonitrile spectrum with the CI background mass set too low (=50 m/z). The 54 ion is visible and has caused a reduction in ionization time. The next figure shows a proper background mass setting for the same conditions (=65 m/z).



CI Background Mass Set Too Low.



CI Background Mass Properly Set.

Determining the Ejection Amplitude

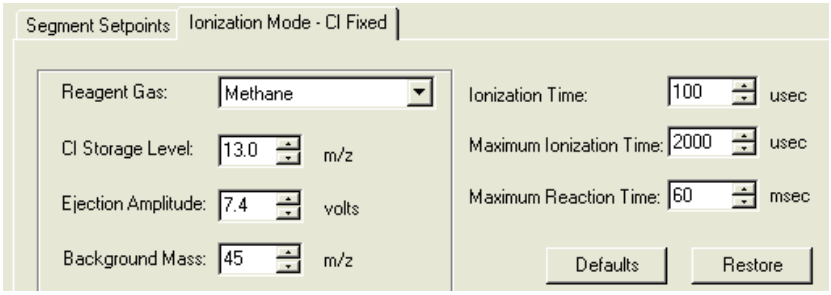
The proper setting for the Reagent Ion Eject Amplitude removes EI generated fragments but does not affect the reagent ions.

To determine the proper ejection amplitude, do the following:

1. Connect and adjust the CI reagent gas.
2. Click the CI Gas control on the System Control.
3. Turn on the trap and observe the spectrum over the scan range specified in the acquisition method. Do not adjust CI gas.
4. Temporarily set the CI background mass to a value below that of the highest mass reagent ion. Record the previous value so you can restore it when you finish with this procedure.

5. Adjust the Ejection Amplitude until the reagent ion starts to be diminished.
6. Restore the CI background mass and verify that no reagent ions remain.

CI with Fixed Parameters



Manually set the reaction parameters normally set by Auto Control. The MS uses the Ionization Time entered in the method editor. The reaction time is determined as follows:

$$\text{ReactionTime} = \frac{\text{MaximumReactionTime}}{\text{MaximumIonizationTime}} \text{x} \textit{Set}\text{IonizationTime}$$

where the maximum reaction and ionization times are entered below the Ionization Time.

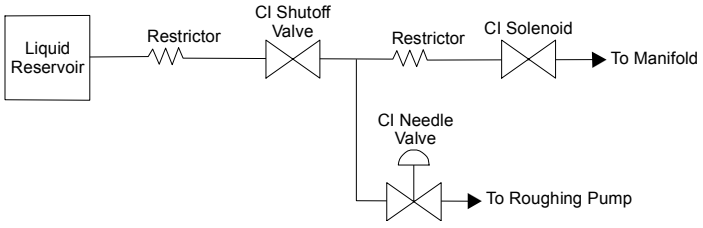
Liquid CI Reagents

Introduction

Liquids can be used as CI reagents. The liquid is placed in a reservoir and connected instead of the CI gas. The vapor pressure of the liquid reagent is usually adequate.

Hardware

The figure shows a diagram of the CI plumbing setup for liquid reagents.



Choice of Liquid CI Reagents

For a liquid to be a CI reagent, it must have moderate vapor pressure and low molecular weight. If the molecular weight is too high, there may be problems

seeing low molecular weight analytes because they are excluded as the reagent ions are ejected. If the vapor pressure is too low, not enough reagent enters the MS for effective CI operation. Remedy this by passing a stream of helium through the reagent vial. This strategy is successful with water.

Use the following as liquid CI reagents:

- Methanol
- Dimethyl ether
- Dimethylamine
- Acetonitrile
- Diethyl ether
- Carbon disulfide
- Water (with a helium stream)

Setting CI Parameters for Liquid Reagents

Set the CI Storage level low enough to store the CI reagent ions.

Set the CI background mass to a level high enough that reagent ions do not appear in the CI spectrum.

Set the Reagent ion eject amplitude between 7.4 and 12.5 volts. As a starting point, use the following values:

Mass	Eject Amplitude
<20	7.5
21-50	9
>50	12.5

Adjust the value as necessary to eject ions above the highest reagent ion and not eject the ions from the reagent.

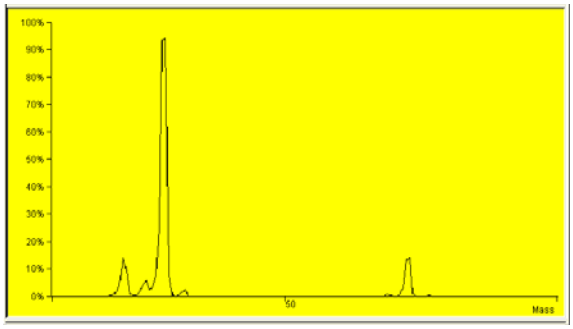
Suggested CI Parameters for Liquid CI Reagents

Reagent Liquid	Acetonitrile	d3-Acetonitrile	Methanol
CI Storage Level (m/z)	19	19	19
Ejection Amplitude (v)	15	15	15
Background Mass (m/z)	65	65	55
Target TIC	5000	5000	5000
Maximum Ionization Time (usec)	2000	2000	2000
Maximum Reaction Time (msec)	40	20	40
Prescan Ion Time (μsec)	100	100	100

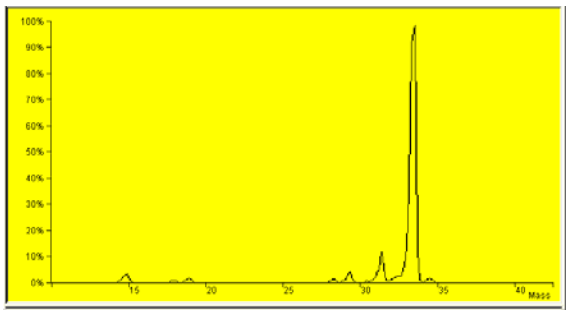
Setting the Reagent Pressure for Liquid CI Reagents

To set the reagent pressure:

1. Connect a liquid reagent reservoir containing the chosen liquid to the liquid reagent inlet block.
2. Open the CI needle valve 6-7 turns counterclockwise.
3. Click the CI Gas Control on the System Control and allow the vapor flow from the reservoir to equilibrate. If, after several minutes, there is not enough CI gas entering the trap, further open the needle valve (clockwise).
4. While observing the spectrum, use Adjust CI Gas to turn the CI needle valve to change the amount of reagent entering the trap until the resolution between M and M+1 just starts to degrade. For best results when using acetonitrile, use a filament emission current of at least 20 μA and maintain at least a 50% valley between m/z 41 and m/z 42.



Properly Adjusted Acetonitrile Reagent Spectrum



Properly Adjusted Methanol Reagent Spectrum

Adjusting CI Reagent Gas Pressure

When installing a new supply of reagent gas, adjust the pressure of the CI reagent gas. After the reagent gas pressure is adjusted, check the pressure at least once every day.

Adjust or check the reagent gas pressure using Adjust CI Gas in System Control.

Checking the CI Reagent Gas Pressure

With methane as the reagent gas, observe the spectrum and adjust the pressure so that:

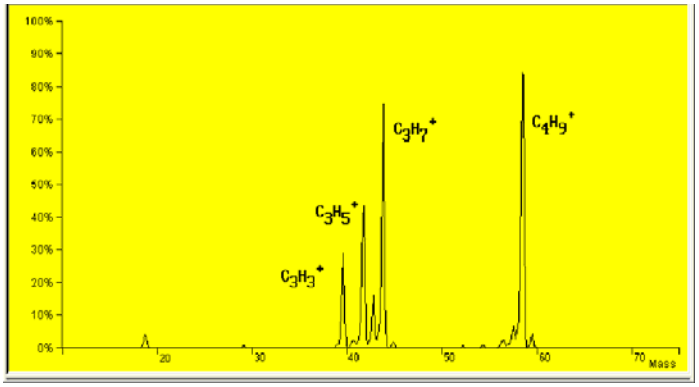
- the ratio of the peak heights at mass 17 (CH_5^+) to mass 16 (CH_4^+) is about 10:1
- the ratio of the peak heights at mass 17 to 29 ($C_2H_5^+$) is about 1:1
- and mass 41 ($C_3H_5^+$) is visible.

If using isobutane or ammonia, do the same procedures to adjust and to check the reagent gas pressure, with the following modifications:

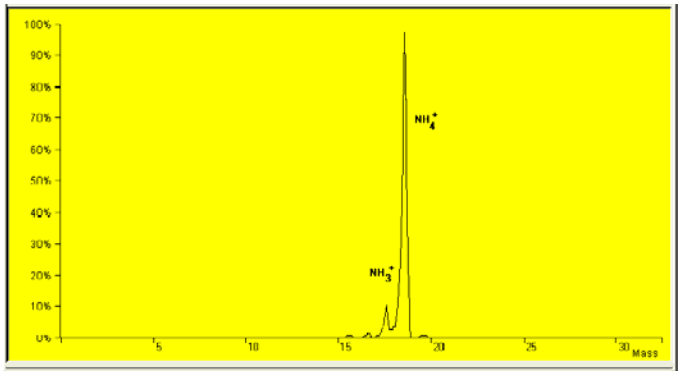
Isobutane: Observe the spectrum and adjust the pressure so that the ratio of the peak heights at mass 57 [$(CH_3)_3C^+$] to mass 43 [$(CH_3)_2CH^+$] is about 1:1.

Ammonia: Observe the spectrum and adjust the pressure so that the ratio of the peak heights at mass 18 [$(NH_3)H^+$] to mass 17 (NH_3^+) is about 10:1.

Following these guidelines, the reagent gas pressure in the ion trap is approximately 1 x 10^{-5} Torr to 2 x 10^{-5} Torr (about 1.3 x 10^{-3} to 2.6 x 10^{-3} Pa).



Reagent Ion Spectrum for Isobutane



Reagent Ion Spectrum for Ammonia

CI Tune

In CI, as in EI, the MS is tuned to achieve the best combination of maximum peak height (sensitivity), optimum resolution of peaks, and smooth peak shape. In addition, as in EI, the key to proper CI tuning is to optimize the number of ions in the ion trap:

- not enough ions, sensitivity suffers
- too many ions, resolution and peak shape suffer.

In CI, the two main factors that affect the number of ions are the ionization time and the reaction time. (The filament emission current is an important third factor.)

The number of reagent ions formed is proportional to the ionization time. The number of sample ions formed is proportional to the reaction time.

To tune the MS for CI, tune and calibrate using System Control Auto Tune. You do not need to run a different automatic setup, tuning, and calibration program for CI. The setup parameters and mass calibration established for EI are satisfactory for CI.

Low and High Pressure CI

Conventional high pressure CI source requires reagent gas pressures on the order of 1 Torr. High pressures are necessary because the residence time of ions is very short, about 10^{-5} seconds. Higher pressures generate the largest number of reagent ions necessary for chemical ionization.

The ion trap accumulates reagent ions and holds them from 1 to 128 milliseconds. The longer residence time can use a lower reagent gas pressure (ca. 10^{-5} Torr) to produce a large population of sample ions.

The practical advantages of low-pressure CI are:

- No need for an expensive vacuum pumping system for the large amounts of reagent gas
- Low consumption of expensive high-purity reagent gas
- Minimal contamination of the ion source
- The potential of alternating EI and CI scans without the compromises in spectral quality seen in high-pressure sources
- Very good CI sensitivity in the full-scan mode
- Liquid reagents are easy to use

MS Ion Preparation

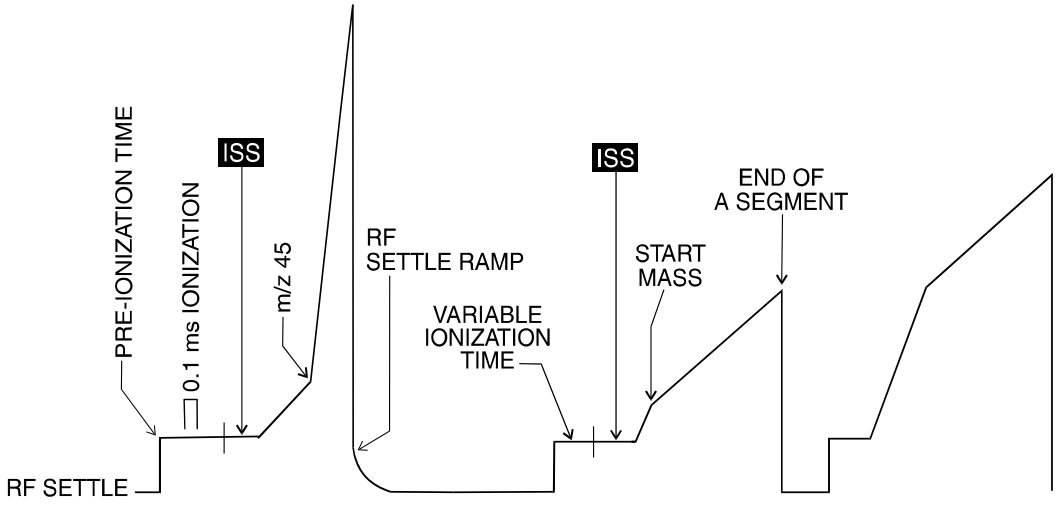
Ion Preparation

The two basic functions in mass spectrometry are ion creation and ion analysis. For some applications, the ability to manipulate the ion population after ion creation but before ion analysis through such techniques as selective storage or dissociation may be advantageous. The ion trap accomplishes it using an ion preparation method (IPM), which modifies the scan function. Advantages associated with IPMs are reduction of noise, increased selectivity, and so on.

Intermediate Scan Segments (ISS)

Ion peparation introduces intermediate scan segments (ISSs) into the basic rf scan function. These permit customization of the prescan and analytical scan(s) for both electron and chemical ionization.

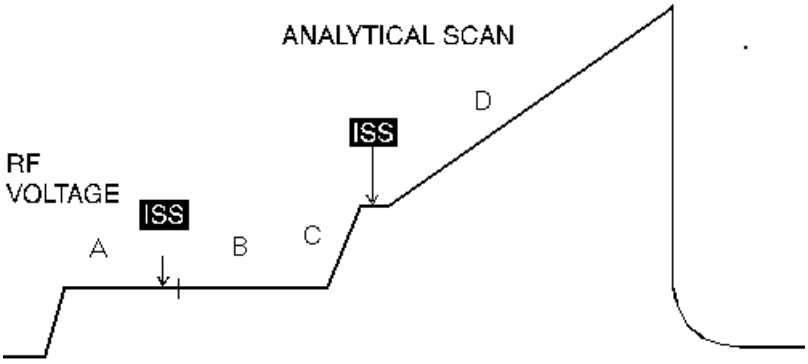
For electron ionization (EI), ISS insertion occurs between creation of the ions (ionization) and ion analysis. Electron ionization uses the automatic gain control (AGC) scan function, which consists of a prescan and up to four analytical scans. As seen in the figure, the prescan and analytical scans include ionization periods, ISSs, and six rf voltage ramps (only two ramps displayed) over a user-defined range.



Automatic gain control scan function with intermediate scan segments

CI has two steps, ionization and reaction. Insert ISSs in the ion preparation following one or both segments of the scan function. CI uses the previous scan for ion control.

The following shows the analytical scan with an ionization period, a reaction period, ISSs, and an rf voltage ramp for mass analysis.



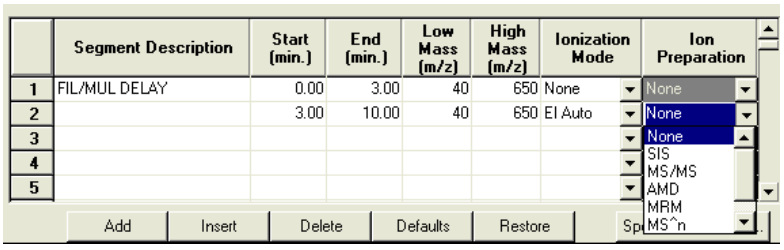
A. Reagent gas ionivation time, as determined by the previous scan.
B. Reagent gas reaction time, as determined by the previous scan
C. Ejection of reagent gas ions.
D. Acquisition of CI mass spectrum

Each intermediate scan segment is defined by the following parameters:

- Duration (in time) of the segment
- Beginning rf storage level
- Ending rf storage level
- DC voltage
- Waveform applied to the end cap electrodes
- Amplitude of the waveform
- States of two auxiliary outputs (ON or OFF)
- State of axial modulation signal (ON or OFF)
- State of the electron multiplier (ON or OFF)

Modify the ionization portion of the scan function to a waveform and rf modulation. Modify the reaction period to include a waveform.

Specifying the Ion Preparation Parameters



The ion preparation parameters control how the EI or CI scan functions are modified for preparing the ions for scanning. They control which ions are ejected,

are retained, and undergo dissociation (CID). Your input and the technique determine how the scan function is constructed and the custom waveforms are created.

SIS Theory of Operation

Use Selected Ion Storage (SIS), to accumulate or store specific ions. Success with this technique requires no excessive space charge build up. Optimum mass resolution is achieved by controlling the number of ions in the trap. When the concentration of background matrix or co-eluting compound is large compared to the target compound, Automatic Gain Control (AGC) maintains the correct number of ions in the trap by reducing the ionization time. However, this also reduces the number of target compound ions for analysis.

SIS ejects unwanted ions from the trap. SIS enriches the sample ions relative to the unwanted matrix ions by ejecting the latter throughout ionization. The unwanted ions are ejected from the trap by resonant ion ejection.

Trapped ions have a characteristic, or secular, frequency of oscillation. This frequency depends on the mass of the ion and the amplitude of the fundamental storage rf field. An ion's secular frequency increases with increasing storage rf voltage, and decreases with increasing mass.

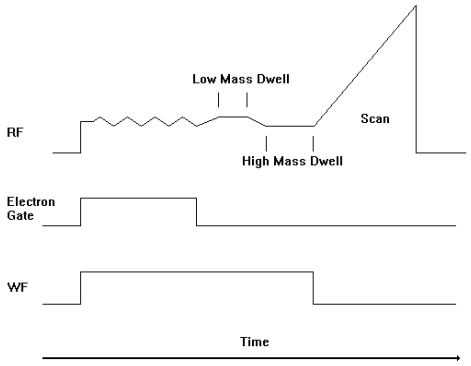
Normally, mass scanning results from the application of a single supplemental dipole field to the end caps of the ion trap, and the application of a linear frequency increase of rf voltage. As the rf voltage is increased, the ion's secular frequency increases until it matches the frequency of the applied supplemental field. At that point, resonance occurs and the ion absorbs energy from the external field. The amplitude of the ion motion increases, and continues to increase until the ion is ejected from the trap and the ion is detected.

Resonant ion ejection may be used to eject multiple ions in a fixed rf storage field by applying multiple frequencies to the end caps. One method of applying multiple frequencies is using a broadband multifrequency waveform. The multifrequency waveforms used in SIS includes the frequencies required to eject the unwanted ions from the trap without affecting desired ions.

Initially, specify the mass window of ions to storage. Because each mass has a unique secular frequency at a given storage rf voltage, it is possible to construct a waveform that does not include frequencies near the secular frequencies of the desired ions. The resulting waveform consists of a distribution of discrete frequencies with missing frequencies, called notches, that correspond to the frequencies of the desired ions.

Modulation (the periodic increase, then decrease) of the storage rf increases and decreases the secular frequencies of the ions in the trap. Thus, the unwanted ions may be brought in and out of resonance with frequencies in the applied supplemental waveform, so that unwanted ions are ejected and desired ions are accumulated.

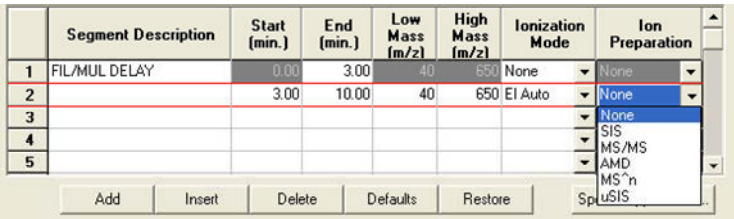
The following figure is a timing diagram of the SIS scan function. Ionization begins when the electron gate is turned on and electrons enter the trap. At the same time, the supplemental waveform (WF) is turned on, and ion ejection begins. With the electron gate and waveform both on, the amplitude of the rf trapping field is modulated to vary the secular frequencies. Application of the waveform and rf field modulation continues for another cycle after the electron gate is turned off. This ensures that all remaining unwanted ions are ejected.



Selected Ion Storage (SIS) Parameters

NOTE: The Ion Trap must be calibrated for optimum performance. Before running any SIS methods, see the MS Workstation Tutorial Manual for Calibration of SIS.

To view the SIS parameters, click SIS from Ion Preparation.

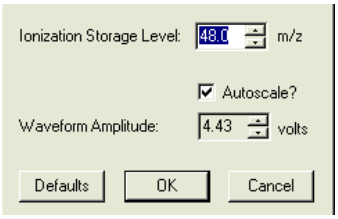


Under Storage Mass Ranges, enter the low m/z integer mass and the high m/z integer mass for each mass window to be stored. Enter up to five mass ranges. The default parameters permit any mass range from 53 m/z to 650 m/z to be stored, with a storage rf of 48 m/z.

Under Ejection Masses, click Ion Mass, click Add, and enter the integer mass(es) of those ion(s) to be ejected, along with the corresponding amplitude(s) as percentages of the amplitudes that would normally be used in a SIS ejection waveform. Enter up to five masses to eject. The Amplitude range is 10% to 200% with a default of 100%.

Customize SIS

Click Customize in the Ion Preparaton SIS tab to cutomize SIS method and enter the Ionization Storage Level to determine the minimum allowable mass.



Ionization Storage Level

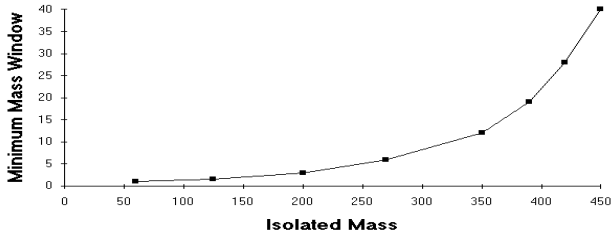
Using the default storage rf level of 48 m/z, the minimum low mass that can be entered is 53 m/z (48 + 5 m/z).

Allowable Storage Mass Range: (storage rf + 5) < mass < 650 m/z.

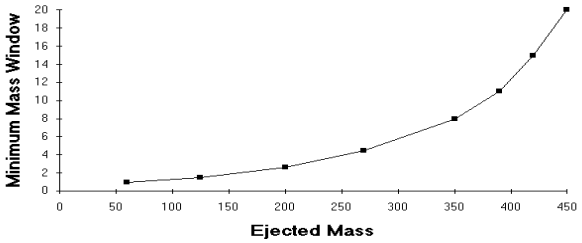
Default = 48 m/z.

The lowest storage rf level that can be entered is 20 m/z, which permits a minimum low mass of 25 m/z to be acquired.

The following figure shows the relationship between the minimum mass window that can be stored and the isolated mass. Unit mass isolation can only occur at low masses. At higher masses, a range of ions is stored even when a single mass is entered.



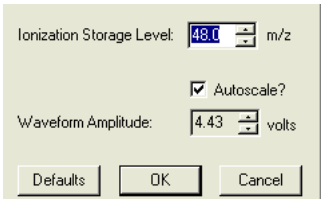
As the following figure shows, the window of ions ejected depends on mass. A single mass can only be ejected at low mass values. If a single high mass value is entered, a range of ions is ejected.



Autoscale Waveform

With default operation (Autoscale = ON), the SIS waveform amplitude is automatically scaled as a function of the frequency components and storage rf voltage selected.

NOTE: Optimize the amplitude of the waveform. Use the method described in the MS Workstation Tutorial Manual, Calibration of SIS or manually increase or decrease the waveform amplitude.



To manually specify the waveform amplitude, deselect Autoscale. Enter the \desired Waveform Amplitude in volts.

Range: 0 ≤ amplitude ≤ 60.00 volts. Default = 15.00 volts.

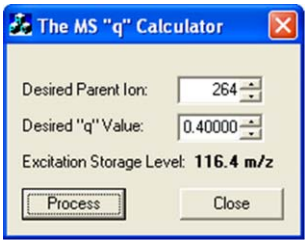
Tips for Using SIS

To obtain the best results when using the SIS application, do the following:

- When selectively storing ions easily fragmented by collision-induced dissociation (CID), use wide mass isolation ranges and low amplitude waveforms.
- As the frequency notches narrow and the voltage of the frequency components increases, the desired ions acquire sufficient energy to be dissociate or to be ejected. As a result, a small fraction of these ions may be lost due to dissociation or ejection.
- Use target TIC values less than 10,000 when using SIS applications, especially with a narrow mass window. Values in excess of 10,000 may cause space charge build-up, which can decrease the linear range for quantitation and result in loss of resolution.

The MS “q” Calculator

The MS q Calculator is in all Ion Preparation Options.



Storage rf values are often reported in terms of the Mathieu “q” parameter in the literature. The “q” parameter determines the stability of the percursor ion trajectory. More stable trajectories allow higher excitation voltages to be applied before ions are ejected from the trap. A “q” value of 0.4 provides an optimum yield of product ions. This calculator utility determines the corresponding CID storage rf value (m/z) following the entry of an ion mass (m/z) and desired “q”.

MS/MS: Theory of Operation

Overview

EI has four basic operations in Ion Trap Tandem Mass Spectrometry (MS/MS):

- Ion formation and matrix ion ejection
- Percursor ion isolation
- Product ion formation
- Product ion mass scanning.

CI MS/MS uses a subset of these and it is valuable because it can:

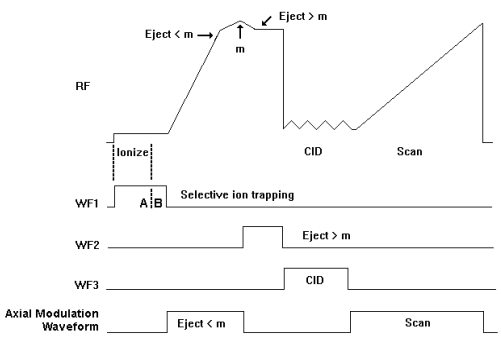
- Optimally fill an ion trap with the selected percursor ion
- Obtain qualitative structural information by forming the product ion spectrum and
- Increase the signal-to-noise ratio by eliminating interfering matrix ions.

Ion Formation and Matrix Ion Ejection

EI ionizes the sample and co-eluting matrix molecules. During ionization, a broadband multifrequency waveform is applied to the end caps to resonantly eject ions below the specified percursor ion mass. This removes unwanted low-mass ions, whose space charge affects the storage efficiency of the percursor ion. Removing most of the space charge improves mass resolution.

After ionization, a second broadband waveform is applied to eject ions with masses above the specified percursor ion mass. This removes most of the remaining unwanted ions. There remains the optimum number of percursor ions with the desired m/z value, along with a few ions with values of m/z slightly above and below it.

This two-step approach only requires one calculation of waveforms. The software can make adjustments to accommodate changes in mass calibration.



Percursor Ion Isolation

Percursor ions can be completely isolated from remaining matrix ions in a two-step process.

- The first step ejects ions with masses below the percursor ion mass by ramping the rf field amplitude with axial modulation applied to the end cap electrodes. This resonantly ejects all ions having masses up to, and including, the mass just below the percursor ion mass. Axial modulation is then turned off.
- In the second step, a broadband multifrequency waveform (WF2) is applied to simultaneously eject all masses above the percursor ion mass. Isolation occurs at elevated rf levels where mass resolution is optimal. Thus, it is possible to achieve unit mass isolation over the entire mass range of the ion trap.

Achieving unit isolation is useful for isolating a single mass in an isotopic cluster, or in separating the percursor ion from interfering matrix ions. This high resolution isolation method is helpful because it is calibrated using the standard mass calibration and uses the same broadband waveform for all masses. Thus, if the system is recalibrated, or if a new percursor ion mass is selected, the waveform does not need recalculation.

Product Ion Formation

Product ions are formed from the percursor ions by collision-induced dissociation (CID). The percursor ions constantly undergo collisions with helium gas in the ion trap. Normally these collisions involve relatively small energies, but if the translational energy of the percursor ion is increased, the collisions may convert the translational kinetic energy to internal vibrational energy.

If the percursor ion acquires enough vibrational energy, one or more chemical bonds may be broken, and ions of lower m/z than the original (percursor ion) m/z formed. The m/z distribution depends on the characteristics of the percursor ion and the amount of energy that converted into internal vibrational energy.

The translational kinetic energy of the percursor ion can be increased by nonresonant excitation or by resonant excitation. In each method, a waveform is applied to the trap. The waveform amplitude the CID excitation amplitude, and the length of time that the waveform is applied is called the excitation time.

Nonresonant Excitation

A low frequency supplemental dipole field is applied to the end caps, resulting in an instantaneous change in the potential energy of the ion in the trapping field.

NOTE: The dipole field is an electric field oriented along the axis of the trap

The force of the trapping field converts the newly increased potential energy of the ion into increased translational kinetic energy. A portion of this kinetic energy is converted into internal vibrational energy during collisions. This process is repeated during each oscillation cycle of the low frequency dipole field.

Resonant Excitation

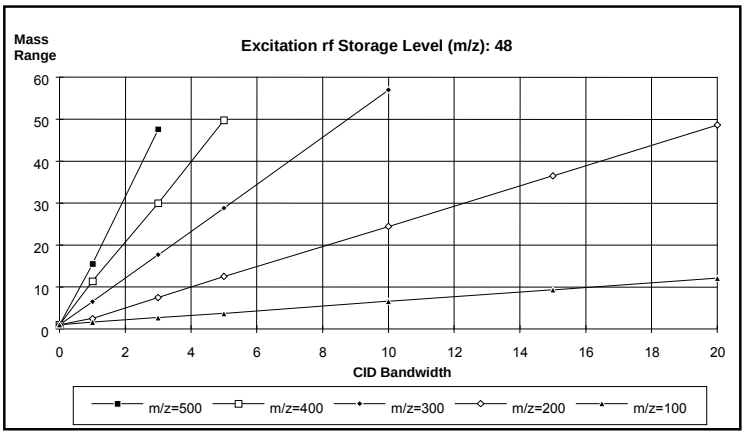
A high frequency supplemental dipole field is applied to the end caps. The frequency must match the oscillation frequency of the trapped ion. The resonant

frequency of the trapped ion depends on ion mass, space charge, rf trapping field amplitude, and other factors. It is difficult to precisely calculate its value. The amplitude of the rf trapping field is modulated over a specified range. As the resonant frequency of the trapped ion depends on the magnitude of the rf field, modulating the rf field amplitude results in a modulation of the resonant frequency of the ion. Modulation of this frequency causes the frequency of the ion to periodically match that of the applied supplemental dipole field. Thus, the energy coupled to ion motion is maximized, and the effects of shifts in the ion resonant frequency are minimized. The effectiveness of the resonant excitation method depends on the mass range over which the rf field is modulated, and the total time spent in resonance.

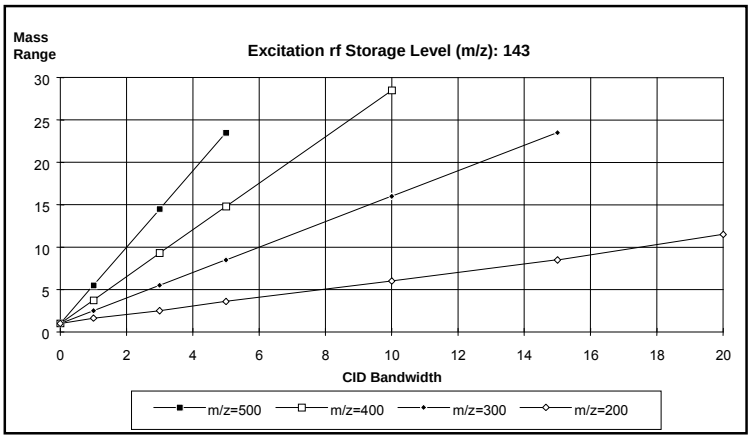
An advantage of nonresonant excitation is that it is not critical to match the applied dipole frequency to that of the ion. As a result, the method is affected neither by electronic drifts, by space charge effects, nor by sample concentration. This results in reproducible product ion spectra, unaffected by changes in the trapping conditions and sample concentration. This is useful with percursor ions that fragment by the breakage of a single weak chemical bond to form highly stable ions containing functional groups that do not undergo significant rearrangements. A disadvantage of the method is that it is not selective with respect to excitation of ions in the trap Therefore, the method cannot be selectively tuned to excite only ions having a particular m/z. The method is also less useful with percursor ions in which multiple chemical bonds are broken and with percursor ions that undergo complex rearrangements following collision-induced dissociation.

The resonant excitation method is selective to the mass range excited. It permits coupling of energy to the motion of an ion with a particular m/z value in a very controlled way. As a result, the rate that the amplitude of the ion motion increases is balanced by the rate that energy is removed by collisions. The ion is not ejected, and energy can be become internal energy by increasing the number of collisions. This is done by increasing the excitation time. It is possible to fragment percursor ions that require the breaking of multiple chemical bonds or undergo significant rearrangements. Periodic modulation through ion resonance results in an averaging of the energy coupled into the ion motion and provides a reproducible product ion spectrum, even with changes in concentration. A disadvantage is that the modulation range and CID bandwidth, in addition to the excitation time and CID excitation amplitude need to be optimized.

Changing the CID bandwidth permits simultaneous excitation of ions within a range of masses. As CID bandwidth increases, the corresponding mass range also increases. At a given CID bandwidth, mass range increases with increasing ion mass, and decreases with increasing excitation rf storage level.



Mass range vs. CID bandwidth for an excitation rf storage level of 48 m/z



Mass range vs. CID bandwidth for an excitation rf storage level of 143 m/z

At a storage level of 48 m/z and a CID bandwidth of 4 kHz, the mass range increases from 3 to 40 m/z when the percursor ion mass increases from 100 to 400 m/z. Given a percursor ion mass of 400 m/z and a CID bandwidth of 4 kHz, the mass range decreases from 40 m/z for a storage level of 48 m/z to a range of 12 m/z for a storage level of 143 m/z.

The amount of energy converted to internal energy in the percursor ion depends on the number of collisions (excitation time), the relative energy of the collisions (CID excitation amplitude), and the rate that the internal energy is removed by collisional deactivation (excitation method). Collision-induced dissociation is always in competition with ion ejection. If the CID excitation amplitude selected is too large, the percursor ion is ejected to the trap electrodes before it can collide with background helium atoms. If the CID excitation amplitude selected is too small, the energy of the percursor ion will not exceed the internal energy threshold required to break the chemical bonds and form product ions. This is because energy is constantly being removed by low energy collisional deactivation. Therefore, the CID excitation amplitude and the excitation time are used to optimize the CID process with an appropriate excitation method.

Product Ion Mass Scanning

After the formation of the product ions by collision-induced dissociation, a single rf ramp is used with the axial modulation field to resonantly scan ions from the trap into the electron multiplier. This generates the product ion spectrum.

Chemical Ionization

CI is another way to fill the ion trap. The ion formation and matrix ion ejection steps described for EI are modified. The addition of the three subsequent MS/MS steps; percursor ion isolation, product ion formation, and product ion mass scanning, into the basic CI scan function (following the ionization and reaction steps) creates the CI-MS/MS scan function.

EI/MS/MS and CI/MS/MS Automatic Space Charge Control

Space charge control for EI/MS/MS and CI/MS/MS occurs by forming ions during a fixed ionization period. Ion formation is the same for EI and CI. After ion formation, all ions outside of the specified isolation window are removed from the trap. The ions are scanned from the trap at the normal scan rate.

Summary

The analytical scan uses ionization, percursor ion isolation, product ion formation, and product ion mass scanning. With automatic space charge control, the number of percursor ions in the isolation window determines the ionization time to maintain the optimum number of ions in the trap.The total ion space charge level is held constant as the sample and matrix levels change. Maintaining a constant level of percursor or product ions in the analytical scan results in consistent, reproducible product ion spectra.

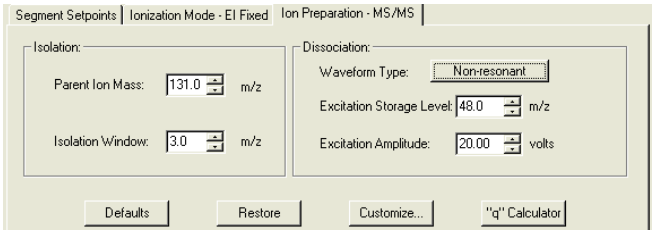
Lower target values may be required to prevent space charging effects. Based on the isolated percursor ion, the following target values are recommended.

Percursor Ion	Target
$60 < m/z < 150$	10000
$150 < m/z < 500$	5000
$500 < m/z < 650$	2000

Additionally, change the EI-Auto PreScan ionization time from the default value. When MS/MS ion prep is selected the ionization time automatically changes to 1500 µsec.

The MS/MS Ion Prep Method

MS/MS Software Parameters



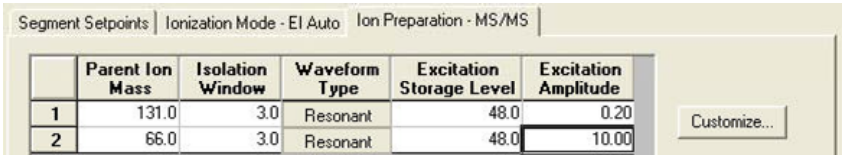
In the Isolation area, enter the Parent Ion Mass (m/z), from 50 to 650 m/z.

NOTE: Integer mass values may be used if the mass isolation window is greater than 1.5 m/z. If the window size is less than 1.5 m/z, or if the mass defect of the percursor ion is greater than approximately 0.3 m/z, use the exact fractional mass.

In the Isolation area, enter the Isolation Window (m/z). The full mass isolation range is 1.0 to 14.0 m/z; the actual range is mass dependent. The default value is 3.0 m/z. Integral and fractional mass isolation windows are both accepted. If mass isolation windows smaller than 1.5 m/z are used, enter the exact mass of the percursor ion in Percursor Ion Mass.

NOTE: When first developing a method, start with a mass isolation window of 3 m/z to ensure that the ion is centered in the window, e.g., given a percursor ion mass of 502 m/z and a mass isolation window of 3 m/z, ions of masses 501, 502, and 503 m/z would be isolated. If there is a need to reduce the window because of interfering ions, do this in a later step because the customized parameters may require optimization.
NOTE: Some ions are easily dissociated during the isolation step. Therefore, increasing the window reduces ion loss by dissociation at the expense of selectivity.

In the Dissociation area, select the Waveform Type. Non reasonant is easier and often used before reasonant.



Excitation Storage Level

Definition: the rf storage level in m/z when the dissociation waveform is applied after isolation.

The excitation storage level range depends on the percursor mass, but the storage level must be more than 2 mass units below the lowest product ion value. The default value is 48 m/z for both resonant or nonresonant modes.

Use the "q" Calculator to determine excitation storage levels.

NOTE: Set the excitation storage level to avoid ejection of the lowest mass product ion. If, a percursor ion of 403 m/z dissociated to product ions with m/z values of 350, 200, and 131, do not use a storage level value above 126 m/z.

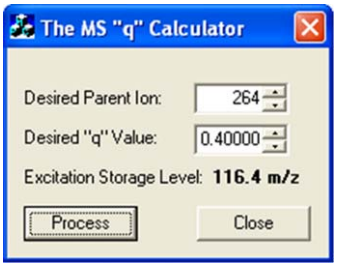
Excitation Amplitude

The amplitude range for nonresonant excitation is 0 to 100 volts. For resonant excitation, the range is 0 to 60 volts. The default values are 20 volts for the nonresonant excitation method and 0.2 volts for the resonant excitation method

NOTE: If the excitation amplitude is too large, the percursor ion and product ion spectra are absent because both ions are ejected from the trap. If the value is too small, the percursor ion spectrum is dominant and the product ion spectrum is weak or missing.

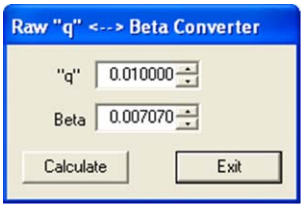
The MS “q” Calculator

For convenience, The MS q Calculator is in all Ion Preparation Options.



Storage rf values are often reported in terms of the Mathieu “q” parameter in the literature. The “q” parameter determines the stability of the percursor ion trajectory. More stable trajectories allow higher excitation voltages to be applied before ions are ejected from the trap. A “q” value of 0.4 provides an optimum yield of product ions. This calculator utility determines the corresponding CID storage rf value (m/z) following user entry of an ion mass (m/z) and desired “q”.

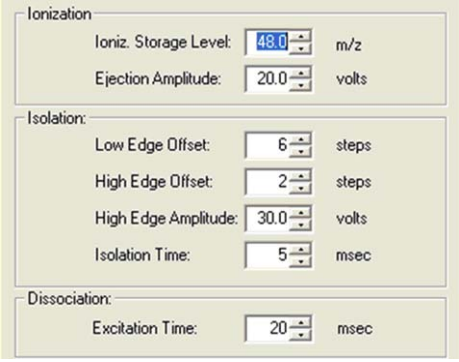
NOTE: Right-click the the “q” calculator button to see the “q” to “β” calculator.



Customize Non-resonant Method

Click Customize to open the MS/MS Ion Prep Method Editor to create a custom MS/MS Ion Prep Method file.

NOTE: Specify the percursor ion mass before opening Customize Parameters.



Customize Parameters has three sections, Ionization, Isolation, and Dissociation.

Ionization

Ionization Storage Level: The m/z value at which the rf is maintained during ionization and the coarse isolation step. The range is 35 to 160 m/z, with a default value of 48 m/z.

Ejection Amplitude: the amplitude (in volts) of the ejection waveform during the coarse isolation step. The default value works for most ions. For ions that are less stable, this value may need to be reduced to minimize the amount of energy imparted to the percursor ion during isolation. The range is from 0 to 60 volts, with a default value of 20 volts.

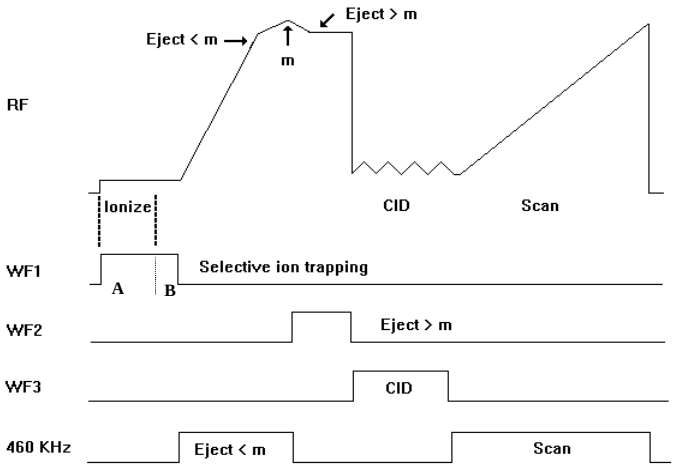
Isolation

Low Edge Offset: The integer value step to optimize the ejection of the mass just below the percursor ion mass. The low edge offset range is 0 to 20 steps. The default value is 6. Low Edge Offset affects the isolation window on the low mass side of the percursor ion. Increasing the value in the positive direction (increasing the default from 6 to 7 steps) opens the isolation window on the low mass side of the percursor ion. Decreasing the offset (decreasing from the default 6 to 5 steps) decreases the window on the low mass side. Adjust the offset to minimize the amplitude of the adjacent masses below the percursor ion. Initially, adjust in 2 step increments. Typically, a 2 step adjustment eliminates the mass below the percursor ion.

High Edge Offset: The integer value step to optimize the ejection of the mass just above the percursor ion mass. The High Edge Offset range is -20 to 20 steps. The default value is 2. High Edge Offset affects the isolation window on the high mass side of the percursor ion. Increasing the offset (from 4 to 5 steps) increases the window; decreasing the offset (from 4 to 3 steps) decreases the window. Adjust the offset to minimize the amplitude of adjacent masses above the percursor ion.

High Edge Amplitude: Amplitude of broadband waveform use to eject masses above the isolated percursor ion. Default is 30 volts.

Isolation Time: The dwell time during which the rf field is held constant in the high mass ejection step.



The isolation time range is 1 to 10 msec. The default time is 5 msec.

Decreasing the Isolation Time to isolate unstable ions. This depends on the amount of percursor ion intensity lost when adjusting the high offset. Adjusting the isolation time is a compromise between the need for long times to efficiently eject the next highest mass during isolation and the need to minimize CID-based percursor ion losses during isolation.

Unstable ions can often be recognized by asymmetric tailing of the mass peak towards the low side of the spectrum during normal mass scanning. In the case of the mass at m/z = 219 from the calibration gas PFTBA, the percursor ion intensity is frequently reduced to the CID intensity of the percursor ion by the broadband waveform used to eject the high mass ions above the percursor ion.

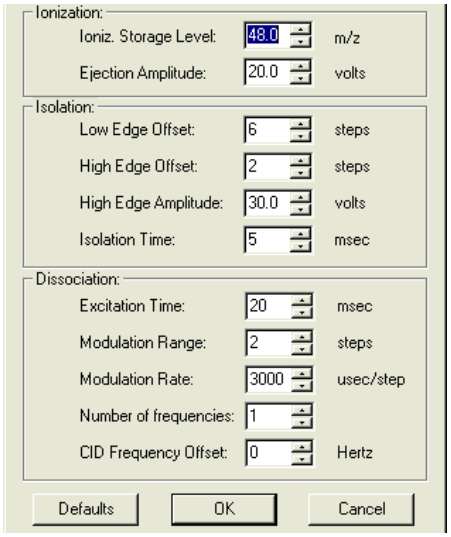
Some of the frequency components in the waveform fall close to the resonant frequency of the percursor ion and may couple energy into the ion motion. Unstable ions can undergo CID at very low energies. By decreasing the isolation time, the percursor ion spends less time in the trap with the waveform present. Stable PFTBA ions that can be used to adjust the isolation parameters are m/z = 69, 131, 264, 464, 502, and 614. Column bleed from polysiloxane phases produces stable clusters of ions at m/z = 181, 207, 281, and 429.

Dissociation

Excitation Time: The excitation time is the time required for collision-induced dissociation (CID) by ion excitation. The excitation time range is 0 to 1000 msec. The default excitation time is 20 msec for both resonant and nonresonant excitation.

Customize Resonant Method

NOTE: Specify the percursor ion mass before opening Customize Parameters.



Customize Parameters has three sections, Ionization, Isolation, and Dissociation.

Ionization

Ionization Storage Level: The m/z value at which the rf is maintained during ionization and the coarse isolation step. The range is 35 to 160 m/z, with a default value of 48 m/z.

Ejection Amplitude: The amplitude (in volts) of the ejection waveform during the coarse isolation step. The default value works for most ions. For ions that are less stable, reduce it. The range of the ejection amplitude is from 0 to 60 volts, with a default value of 20 volts.

Isolation

Low Edge Offset: A fine adjustment for the isolation window to optimize the ejection of the mass just below the percursor ion mass. The low edge offset range is 0 to 20 steps. The default value is 6.

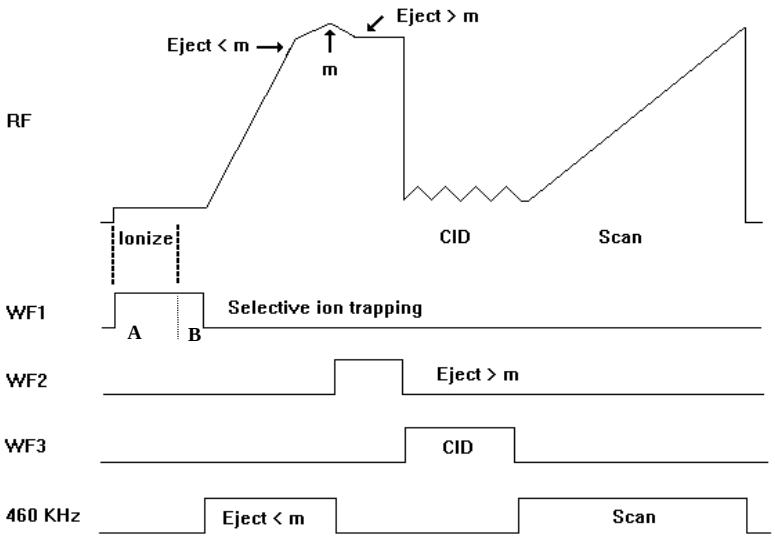
- Large positive values widen the isolation window towards low masses.

High Edge Offset: A fine adjustment for the isolation window to optimize the ejection of the mass just above the percursor ion mass. The High Edge Offset range is -20 to 20 steps. The default value is a function of the percursor ion mass.

- Large positive values widen the isolation window towards high masses.

High Edge Amplitude: Amplitude of broadband waveform used in the two-step isolation to eject masses above the isolated percursor ion. Use the default value for stable ions, and reduce it for unstable ions. The range is 0 to 60 volts with a default value of 30 volts.

Isolation Time: The dwell time the broadband waveform is applied during the high mass elimination step. Use the default value for stable ions, and reduce it for unstable ions. The range is 1 to 10 msec with a default value of 5 msec.



NOTE: For unstable ions, decreasing the isolation time improves the isolation efficiency.

Dissociation

Excitation Time: The time required for collision-induced dissociation (CID) by ion excitation. The excitation time range is 0 to 1000 msec. The default excitation time is 20 msec for both resonant and nonresonant excitation.

Modulation Range: The step range over which the rf storage field is modulated during resonant CID. This modulation greatly reduces any effect of changing secular frequency with concentration. The default is sufficient for exciting a single ion. When trying to excite an isotopic cluster, increase this value and/or increase the CID bandwidth. The range is 0 to 12 steps. The default value is 2 steps.

NOTE: This value is not used if the nonresonant CID method is selected. A value of 0 gives a fixed rf storage field, that is, no modulation

Modulation Rate:The number of microseconds spent at each step. The range is 29 usec to 5600 usec, with a default value of 3000 usec/step. The default value works for most applications.

Number of Frequencies: Enter an odd integer in the range of 1 to 121 for the number of frequencies. A value of 1 generates a single supplementary frequency applied to the end caps. An value of 3, generates three frequencies: the resonance frequency and frequencies 500 Hz above and below.

CID Frequency Offset : Offseting the dissociation frequency is helpful for some applications. The CID frequency can be adjusted between $\pm$ 3000 Hz.

Tandem Mass Spectrometry (MS/MS)

Customizing Percursor Ion Isolation

To optimize percursor ion isolation by reducing the isolation window:

1. Build a method with a mass isolation window of 3 m/z, an excitation time of 0 msec, and a CID (excitation) amplitude of 0 volts. This permits observation of the isolation of the percursor ion without the influence of CID. Use the exact fractional mass of the ion for the percursor ion mass.
2. Use a fixed sample source, such as the perfluorotributylamine (PFTBA) calibration gas, or the column bleed obtained by raising the gas chromatograph oven temperature to 300 °C.
3. Adjust the isolation parameters to isolate a single ion.

Selecting an Excitation Technique

The sample and matrix determines the excitation technique. Begin your analysis with nonresonant excitation because it requires less work. If the desired results cannot be obtained, switch to resonant excitation.

Optimizing Nonresonant CID Parameters

To optimize the nonresonant or resonant excitation CID parameters.

1. Determine if the CID (excitation) amplitude was too large or too small.

NOTE: If the CID (excitation) amplitude is too large, the percursor and product ion spectra are absent because they were ejected. If too small, the percursor ion spectrum dominants and the product ion spectrum is weak or missing.

2. Increase or decrease the CID excitation amplitude until the spectra changes. For nonresonant CID, use 10 volt steps; for resonant CID, use 0.2 volt steps.
3. Continue to increase or decrease the CID excitation amplitude, in smaller increments until suitable ion spectra are obtained.
4. Adjust the excitation time in 10 ms steps to optimize the spectra.

NOTE: If the percursor ion is ejected instead of forming a product ion, increase the excitation rf level from 48 to 55 m/z and adjust the CID excitation amplitude. Increasing the rf storage level needs a higher amplitude to dissociate ions. Do not raise the excitation rf level above the storage level of the product ions.

Customizing Resonant Excitation

Using a fixed sample source such as perfluorotributylamine (PFTBA) calibration gas or the column bleed obtained by raising the GC oven temperature to 300°C, follow these steps to customize the resonant excitation method.

1. Reduce the modulation range to 0 steps. The modulation rate has no effect on the spectra, that is the rf storage level is fixed.

2. Adjust the CID excitation amplitude and excitation time as needed, to optimize percursor-to-product ion conversion.

NOTE: If the amplitude is large enough, the percursor ion is ejected. Percursor ion ejection indicates that the CID frequency is properly resonant and that the trap function is correctly calibrated.

3. Increase the modulation range to 2 steps. Alternatively, increase the CID bandwidth by increasing the Number of Frequencies from 1 to 3. This increases the mass range around the percursor ion excited. Several frequencies may be used with or without modulation, and may be useful to excite isotopic clusters.

Automated Methods Development

Automated Method Development (AMD) optimizes CID conditions for product ion formation in a MS/MS method. AMD uses up to 10 different sets of conditions for the same percursor ion.

Set the method for 1 microscan per analytical scan by adjusting the Scan Time. The software calculates the minimum scan time allowed based on the duration of one microscan for the current parameters. This ensures that the maximum number of cycles through the different voltages (scan segments) across each peak is performed.

To use AMD to determine the optimum excitation storage level and excitation voltage, do the following:

Determine the percursor ion and retention time for each compound from an injection using normal EI mode. Build a multi-segment acquisition method, with one segment per compound.

Use the default conditions with Automatic Methods Development to determine the mass of the product ion(s). AMD allows the CID voltage to be incremented on a scan-by-scan basis (25V, 30V, 35V) for up to 10 scans and then repeates the cycle.

After determining the m/z of the product ion, perform the following calculation. Product ion m/z divided by 1.4 = the highest CID rf excitation level. For example, if the product ion is m/z 140, then the rf excitation level must be no higher than 100. This ensures good trapping efficiency of the product ion. The value of 1.4 is a ratio of the “q” ejection value (.908) and the “q” value at Beta(1/3) of 0.63.

Optimize the CID voltage with two injections that use AMD. The first injection can use voltage increments of 10 volts (Nonresonant) or 0.2 volts (Resonant). Lower the voltage increment and optimize the voltage with the second injection.

Determining Optimum Voltage for Nonresonant Excitation

To determine the optimum voltage for nonresonant excitation, do the following:

1. Verify that the percursor ion is isolated without a large intensity loss. Set the excitation amplitude for the scan segment 1=0 volts. Inject the sample and examine the spectra across the peak.
2. Set the excitation rf equal to the lowest mass product ion expected divided by 1.4. If the product ions are not known, start with an excitation rf=48 m/z and an excitation time of 20 ms. Set the AMD method to cycle through excitation voltages using increments of 5 or 10 volts.

NOTE: If a more accurate value is needed, inject the sample and increase the CID excitation amplitude by 2 or 3 volts for each group near the best values found with the 10-volt increments.
NOTE: If the rf level was increased to trap the lowest product ion and a satisfactory number of product ions is not obtained, try another percursor ion or switch to resonant excitation. Some ions are sufficiently stable that they are ejected from the trap before they can acquire enough energy to dissociate. Also try increasing the excitation time.

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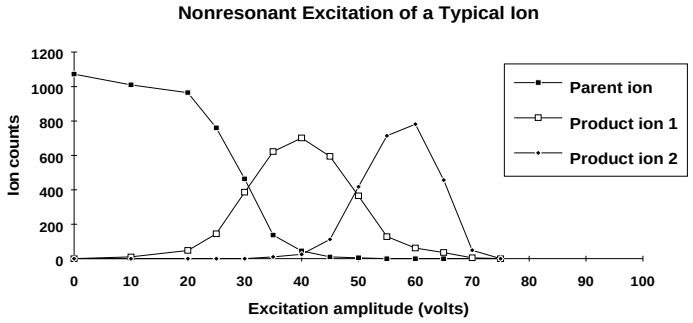
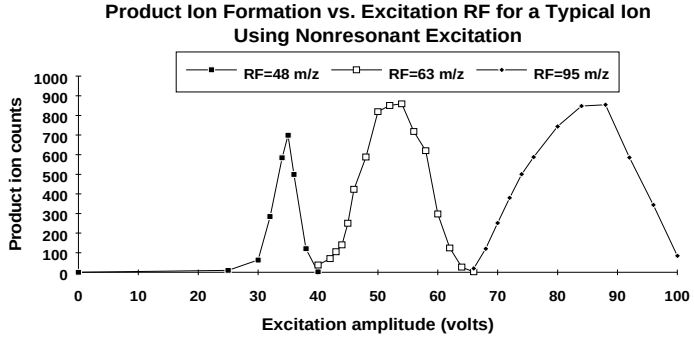
3. Determine the optimum voltage by plotting the product ion intensity data as a function of CID (excitation) amplitude as in the following.



4. Determine the optimum rf level by plotting the product ion intensity data as a function of CID (excitation) amplitude for different rf levels as in the following.

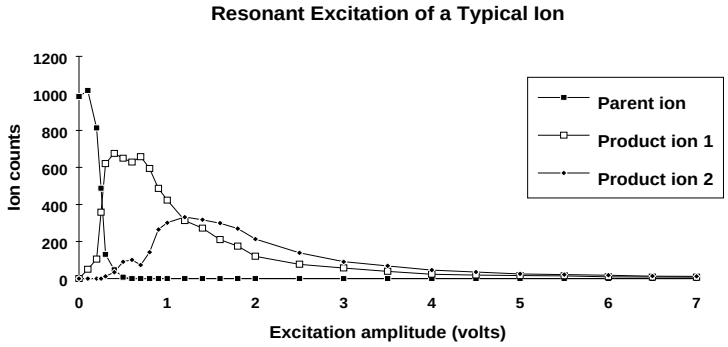


NOTE: The maximum yield of product ions shifts to higher CID (excitation) amplitudes as the rf level is increased.

Determining Optimum Voltage for Resonant Excitation

To determine the optimum voltage for resonant excitation using AMD while injecting the percursor compound, do the following:

1. Set the excitation rf equal to the lowest mass product ion expected divided by 1.4. If the product ions are not known, start with rf=48 m/z and an excitation time of 20 ms. Set the AMD method to cycle through excitation voltages using increments of 0.2 or 0.5 volts.
2. Determine the optimum voltage by plotting the product ion intensity data as a function of CID (excitation) amplitude as displayed in the following.



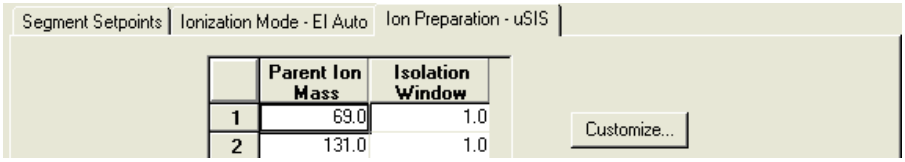
This is a typical breakdown curve for resonant excitation with default parameters.

MS/MS

Do multiple reaction monitoring by adding lines of different percursor ions masses and different dissociation parameters. The limit is nine.

Unit Resolution Selected Ion Storage

Unit Resolution Selected Ion Storage (uSIS) can isolate up to 9 ions with unit mass isolation. This is useful where the standard SIS window is too large.



Use uSIS when narrow mass ranges are required. The allowed storage windows vary up to 3u at m/z less than 80 and up to 14u at m/z 420 and above.

If larger ranges are needed, use SIS.

MS/MS/MS

MS^3 uses two percursor ions for sequential dissociation. The additional dissociation step can increase selectivity of analyte versus background or can provide additional structure information.

First, determine the optimized conditions for MS/MS of the first percursor ion. AMD will make this process go faster.

Then optimize the conditions for dissociation of that product ion (enter under percursor Ion 2). You may need to make sequential injections using the MS^3 method. If the second generation product ion is in the original EI or CI spectrum, then use AMD to find the optimum conditions.

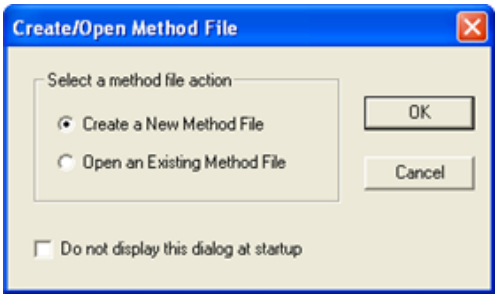
Using MS Methods

Overview

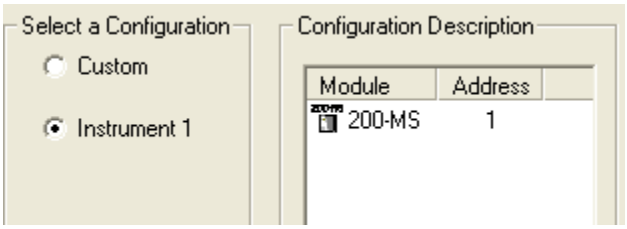
Use Method Builder to view and edit methods. Open it from MS Workstation Toolbar or the startup.mth button. The method can be opened from the System Control bar by clicking the startup1.mth button.

Creating a New Method

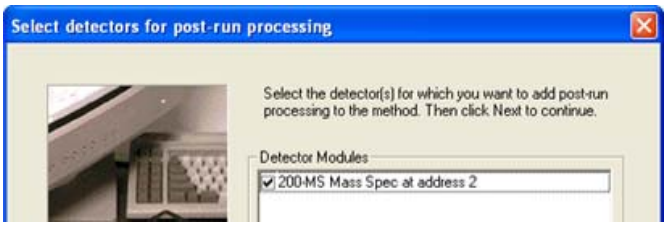
1. Click Method Builder on the MS Workstation Toolbar, to open the following.
2. Select Create a New Method File and MS Workstation guides you.



3. Select Instrument **1** for the 200-MS module, and then click **Next**.



4. Select the 200-MS, and then click Next.

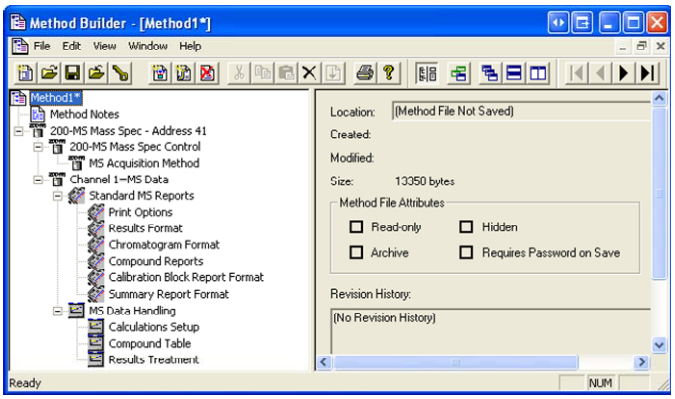


Select **Channel 1** and the listed processes, and then click **Next**.

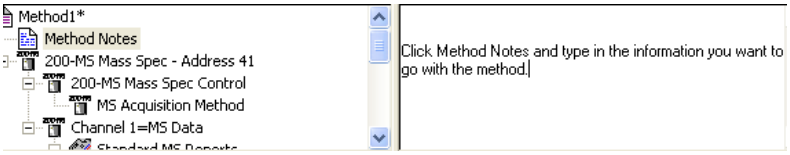
MS Workstation creates a Method with sections containing default values. Edit these parameters.

Method Builder

Select a method section from the tree to view and edit it.



Method Notes



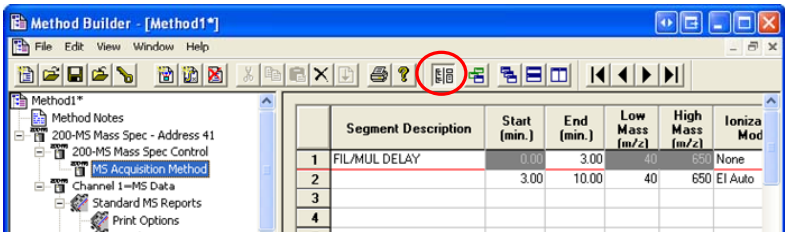
The first item in the Method is the Method Notes section. Method Notes is a form text field. Method Notes are displayed in the File Open dialog boxes used whenever you select a Method.

Method Notes can help explain to the operator when a Method should be used. They can also be used to convey sample preparation information and reminders to refer to specific items in the lab's Standard Operating Procedures.

MS Method Windows

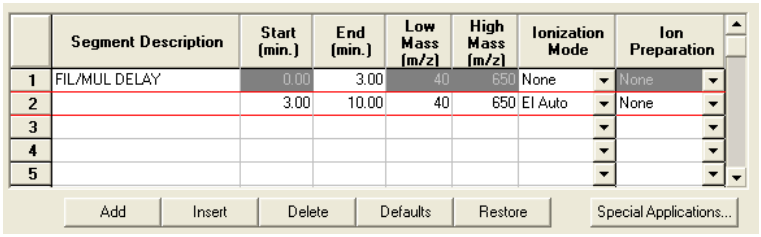
In the Method Directory pane, click MS Acquisition Method. The display on the right shows the MS method. Click the splitter bar separating the Method Directory from the Method Display and adjust the position so that the entire

Method is visible on the screen. Or, hide the Method Directory. On the Method Builder toolbar, click the Show/Hide Method Directory button.



Spreadsheet Editing

A method can have a maximum of 250 segments that are in a spreadsheet.



The spreadsheet options are as follows:

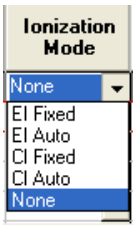
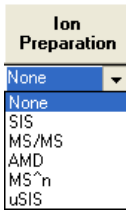
- Click the row number to select a row.
- Click Add to copy the MS parameters of the previous segment, except for the segment description into a row that is added to the end.
- Click Insert to insert a row before the selected row. It will have the same parameters as the selected row.
- Click Delete to delted the selected row.
- Click Default to insert the system default parameter in the current segment.
- Click Restore to insert the segment parameters present when the method was first opened or last saved.

Method Segment 1 is ususally a Filament/Multiplier Delay. This segment is acquired with the filament and multiplier turned off to protect the instrument until after the elution of the solvent peak. The delay time can be set to 650 minutes, although 150 minutes is the recommended maximum. The Ionization Mode is None. If a Filament/Delay segment is not needed, **Delete** the row.

Select the Method Segment 2 **Segment Description** to enter a description.

- Click or tab to **Start** and start time.
- Click or tab to to **End** and enter end time. The range for segment time is from 0.10 to 650.00 minutes.
- Click or tab to **Low Mass** to enter low mass for acquisition.
- Click or tab to **High Mass** to enter high mass value. The mass range is from 10 to 650 m/z.
- Click or tab to **Ionization Mode.** Select from the list.
- Tab to **Ion Preparation** and select from the list.

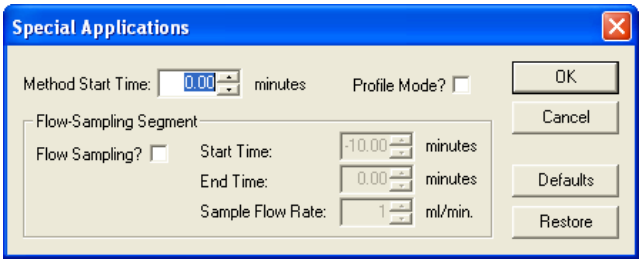
- Select **None** to acquire regular EI or CI spectra.

Ionization Mode Options	Ion Preparation Options
	

Multisegment Chromatogram Time Gaps

In a single acquisition, acquire data in different Ion Modes (EI/CI - Auto/Fixed) and use different Ion Preparation techniques. MultiChro displays each segment independently in the Chromatogram display. There is no connection between the last point in one segment and the first point of the next segment. There is a small time gap between segments. This gap is usually 1.0 ± 0.2 seconds for all acquisition modes except Automated Method Development (AMD) for MS/MS method development. Using 10-segment AMD, the break between segments is about 1.5 seconds.

Click the **Special Application** button.



Specify the data to acquire in Profile Mode (as opposed to Centroid).

NOTE: Data Handling cannot process a data file collected in profile mode.

Also, specify a pre-acquisition flow-sampling period.

The Flow Sampling Segment

The flow sampling segment, designed for air monitoring systems, can be used for other applications. Using the optional hardware to connect the Electronic Mass Flow Controller (EMFC) readout to the MS, permits the actual flow rate to be monitored over the sampling interval and recorded in the data file. The data determines the actual sampled volume and is saved as the flow profile. The Method Start Time includes the time to flush the system, and the sampling time. The sample volume is determined by the specified sample flow rate and the sampling duration (start time - end time). View the theoretical and actual sample volume in the log file. The flow sampling segment is always performed before the other segments, unless its duration is set to zero. Having the flow sampling segment as a separate segment performed before the rest of the acquisition makes the chromatographic retention time independent of the sampling duration:

the data system clock is reset when the sampling is completed. The GC run time is not reset at the end of the sampling segment.

The flow sampling segment is accessed using the **Special Application** button.

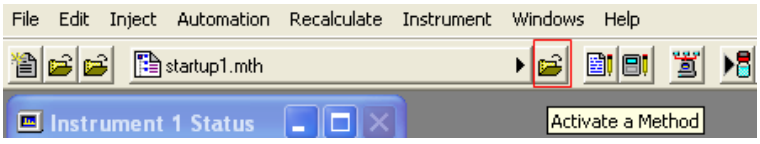
- **Method Start Time**: Flush the system before sample collection begins plus the actual sampling time. Enter a time between -30 to 0 minutes.
- **Start Time/ End Time**: Enter the sampling time, from -10.00 to 0 minutes. If the duration of the segment is set to 0, no flow sampling is done.
- **Sample Flow Rate**: The range is from 1 to 100 mL/min. If the EMFC is in manual mode, the sample flow rate must equal the rate set on the EMFC. If the EMFC is set to auto mode, the sample flow rate specified is downloaded at the start of the injection.

The Startup Method

When you enter System Control and open the MS System Control Window, the Startup1.mth (first time) or the last active Method for 200-MS is activated. The Startup method is a copy of the Default method and can be used to build new control methods. Change the Startup method to use a customized parameters.

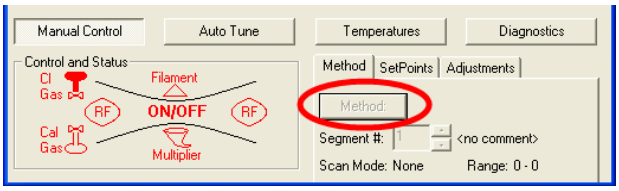
NOTE: The Default method is in the file directory to ensure the a skeletal valid method for the operator. Do not alter this method when developing new methods.
NOTE: While building new methods, click the Defaults button to place instrument valid default values in the section, regardless of the values in the Default.mth.

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



Editing Methods from Status and Control

Click the Method button to load and edit the active Method.



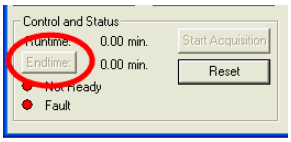
After editing the Method and closing Method Builder, you are prompted to reactivate the Method, which downloads the changes to the MS.

NOTE: If you access the active method from the method editor through the Workstation toolbar, when the method editor is closed or the file saved, reactivate the method in system control. To reactivate the current method, click the button in the System Control toolbar.

Changing Method End Time from Control and Status

During an acquisition, change the end time of the acquisition from the Control and Status window.

1. Click **Acquisition**.
2. Click **Endtime**.

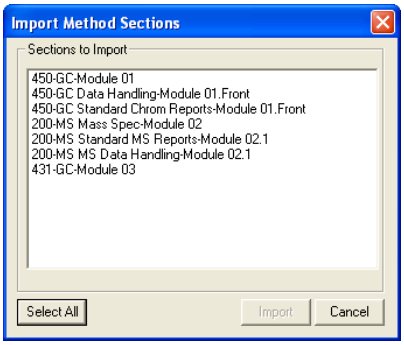


3. Enter the new end time, and then click **OK**.

Importing Method Sections

To copy sections from one method file to another:

1. Open the Method file that you want to edit in Method Builder.
2. Select **Import Section.**
3. Select the file with the desired section.



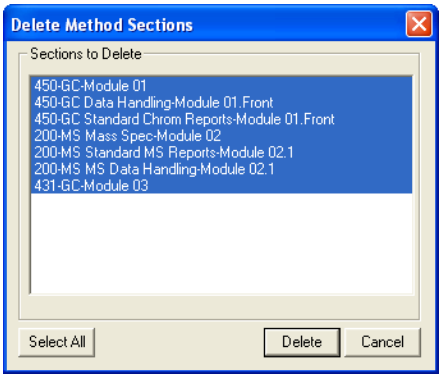
4. Click the sections to import.
5. After selecting the sections, click the Import button to import them. If the Method has sections with the same module address and channel ID, you are prompted to reassign a new module address and channel number to the imported section or overwrite the existing section in the current method.

Deleting Method Sections

To remove sections from an MS Method:

1. Open the Method containing the sections to remove in Method Builder.
2. Click **Delete Section** on the Method Builder Toolbar or select **Delete Section** from the File menu.

3. Click the sections to delete in the box that opens.
4. Click **Delete**, and confirm, when prompted.



Printing the Method

To print a method from Method Builder:

1. Click **Print** on the Toolbar.
2. Select the Method section or sections to printed.

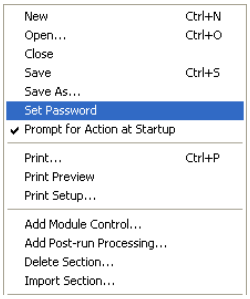
To print from the System Control Toolbar:

4. Click **Active Method Options** on the System Control Toolbar or **Method Operations** on the MS Workstation Toolbar.
5. Select **Print** Method.

Password Protecting a Method

To password protect a method from changes:

1. Cick Set Password on the Method Builder Toolbar or click Set Password from the File menu.



2. Enter the password and then re-enter it for verification.
3. After password protecting a Method the password is required to save changes.

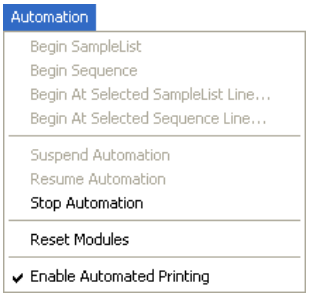
After a Method is password protected, it can be activated and used for instrument control and data acquisition orviewed from Method Builder.

Automated MS Report Generation

Overview

Use the Print actions in the Sequence window to generate automated reports from System Control after each injection or after recalculations.

Disable Automated Report printing during the course of an automated sequence of injections or recalculations. Disabling automated printing from the Automation menu in the Instrument window.



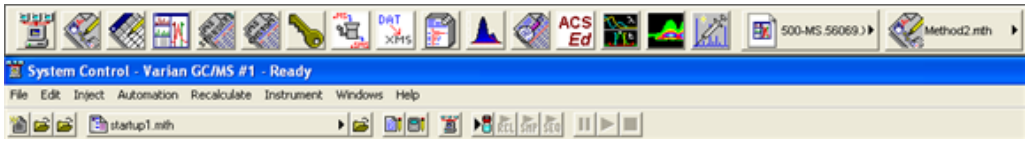
When not checked, report printing is disabled. ASCII file generation is performed, if specified in the Report Method section.

Disabling automated printing is analogous to disconnecting the printer—automation continues but no reports are printed.

Using 450-GC Methods

Overview

Use Method Builder to view and edit methods.



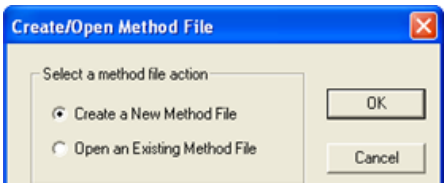
Opens Method Builder and prompts you to create a new method or open and existing one.

View and edit the method on the button.

View and edit the method on the button.

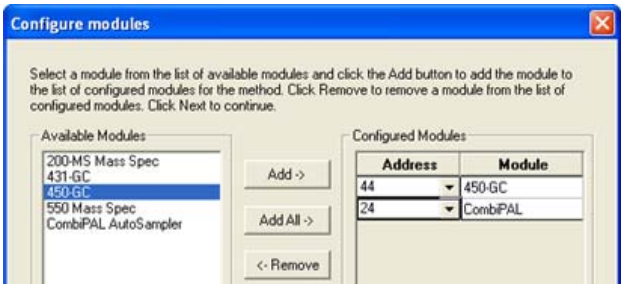
Using Method Builder to Create a New Method

1. Click Method Builder on the MS Workstation Toolbar.
2. Click **Create a New Method File**.

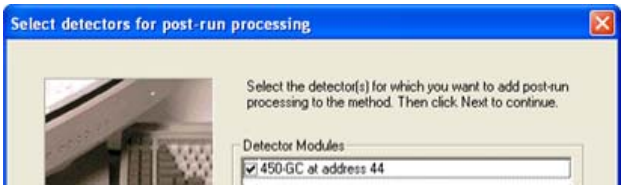


3. Click **Next**.
4. Click Instrument 1 for the current instrument configuration or click Custom to create a Method for an instrument not attached to the MS Workstation.

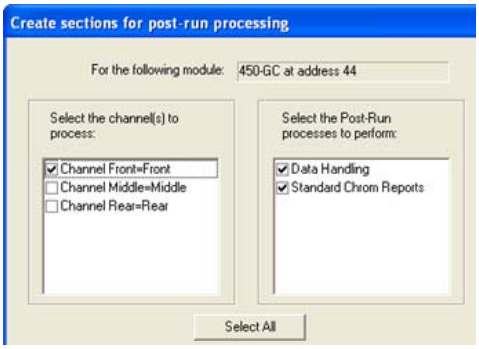
5. Select the modules.



6. Select the detectors for post-run processing.



7. For each detector, select the post-run processing.

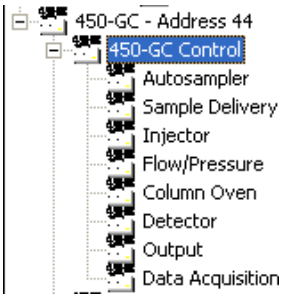


Method Builder creates a Method with default values for the parameters. Edit them for your analysis.

The 450-GC Method Windows

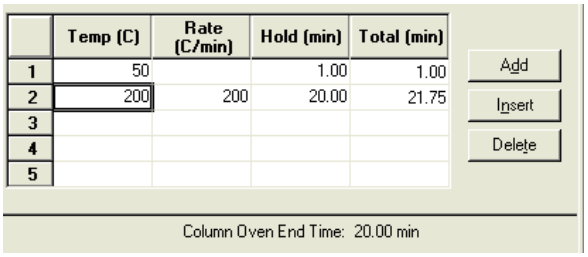
The 450-GC entry specifies the module address. The module Address can be changed so that a Method developed for an instrument using one module address can be easily modified another instrument at a different module address.

The 450-GC Method section contains seven Method windows: Autosampler, Sample Delivery, Injector, Flow/Pressure, Column Oven, Detector, Output, and Detector Information.

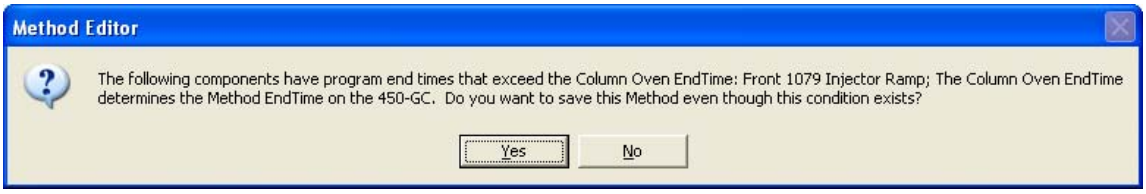


Checking Method End Times

Editing windows, other than the column oven window and data acquisition window, show the current end time of the column oven program below the table.



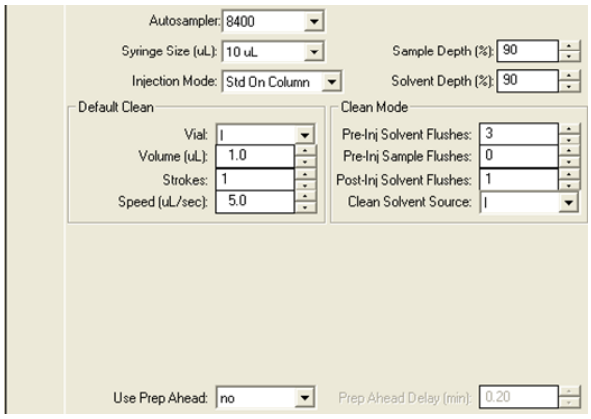
If you enter program end times for components other than the column oven that exceed the column oven end time, the following message is displayed.



When the Method is downloaded to the 450-GC, component program end times that exceed the column oven end time are truncated.

Autosampler Window

The Autosampler window has sampling parameters for the 8400/8410 Autosampler. Use the parameters to select the sampling Syringe Size, the penetration depth for sample and solvent wash Vials (Sample and Solvent Depth), the Default Clean and Clean Modes, and the Injection Modes.



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

Injection Mode

The Injection Mode selection has six injection modes: Standard Split/Splitless, Standard On-Column, Neat, Viscous, Volatile, and SPME (Solid Phase Microextraction). Use the User Defined mode to create a custom one. Select User Defined mode to access all 8400 autosampler parameters.

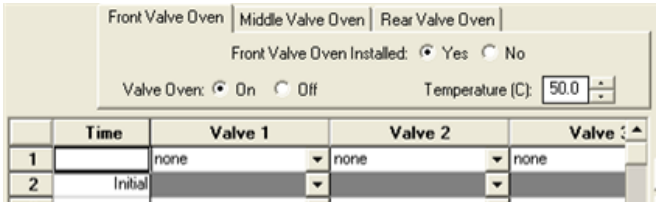
Sample Delivery Window

The Sample Delivery window has the Valve Table Program and up to three Valve Oven Programs (Front, Middle, Rear).

Click Yes or No for Valve Oven.

If a Valve Oven is installed, a Valve Oven switch and a Temperature setting open. Click the installed Valve Oven On or Off.

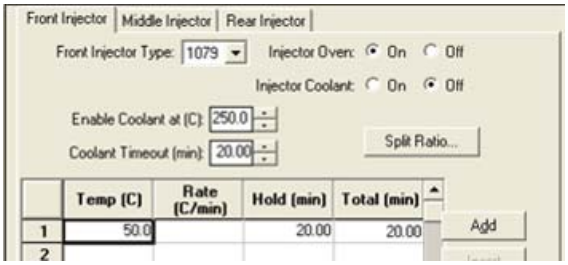
Create a program and specify the isothermal temperature of each Valve Oven.



The first two rows are added automatically. Use the first row to configure each valve to match the GC setup. The second row has the Initial setting for each Valve. Each valve is switched to this setting when the method is activated, and restored to this setting after each run is completed. The following rows contain the programmed settings.

Injector Window

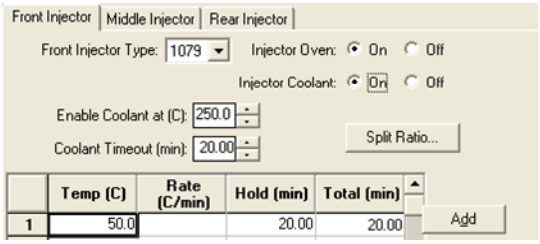
The Injector window has up to three Injector Programs (Front, Middle, Rear). Use the Injector Programs to specify the temperature setpoints of the isothermal 1041, 1061 and 1177 Injectors, and to specify the temperature ramp and split ratio of the programmable 1079 Injector. Select the type of injector at each position, or select “None” if no injector is installed at that position.



1079 Injector

Select a 1079 Injector and an Oven Power switch and a Coolant switch are displayed. Click the installed 1079 injector On or Off.

If you turn the Coolant on, specify the desired **Enable Coolant at** temperature and **Coolant Timeout.**



Build a temperature ramp program to heat and/or cool the 1079 injector.

The first row has 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 run is completed.

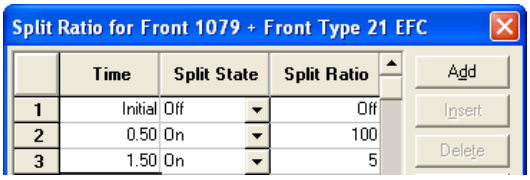
The following rows have the programmed settings for each ramp segments. Each segment ramps to the specified temperature at the specified rate (assuming the rate is achievable), and then hold the temperature for the specified time. Rate, in the first row, is always blank and cannot be edited. Also the Total column cannot be edited.

1079 Split Ratio

If the 1079 Injector is connected to a Type 21 or Type 25 EFC, click the Split Ratio to build the Split Ratio Time Program.

NOTE: You must have already configured the Type 21 or Type 25 EFC in the corresponding position in the Flow/Pressure Section before you can program the split ratio. Specifically, to build a 1079 Split Ratio Program, a Front 1079 must have a corresponding Front Type 21 or Type 25 EFC, a Middle 1079 must have a corresponding Middle Type 21 or Type 25 EFC, and a Rear 1079 must have a corresponding Rear Type 21 or Type 25 EFC.

Use the Split Ratio spreadsheet to build a split ratio time program to control the 1079 injector / Type 21 or Type 25 EFC combination. You can use a spit ratio of 100 after injection to vent the injector of any residual solvent. Use a very low split ratio after flushing to conserve carrier gas.



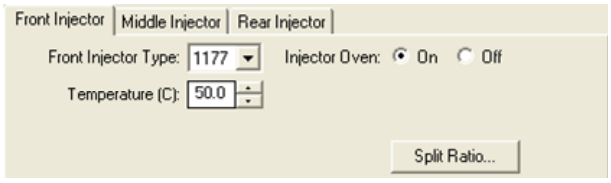
The first row has the Initial Split State and Split Ratio for the 1079 injector. The 1079 equilibrates to this setting when the method is activated, and is restored to this setting when each run is completed.

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

1177 Split Ratio

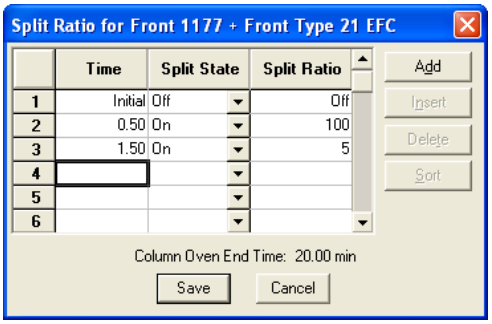
Click the 1177 injector on, and the desired temperature.

If the 1177 Injector is connected to a Type 21 or Type 25 EFC, click Split Ratio.



NOTE: You must configure the Type 21 or Type 25 EFC in the corresponding position in the Flow/Pressure Section before programing the split ratio.
For example, to build a 1177 Split Ratio Program, a Front 1177 must have a corresponding Front Type 21 or Type 25 EFC.

Use the Split Ratio to build a split ratio time program to control the 1177 injector / Type 21 or Type 25 EFC combination. Use a split ratio of 100 after injection to vent the injector of any residual solvent. Use a very low split ratio after flushing to conserve carrier gas.

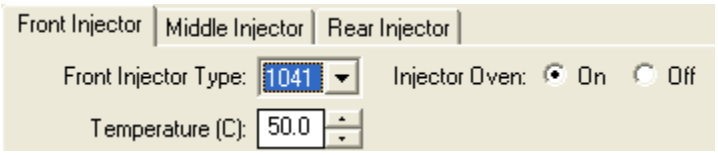


The first row has the Initial Split State and Split Ratio. The 1177 equilibrates to this setting when the method is activated, and is restored to this setting after each run is completed.

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

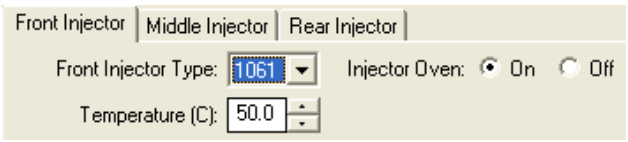
1041 Injector

Selecte the installed 1041, turn it on, and set the temperature.



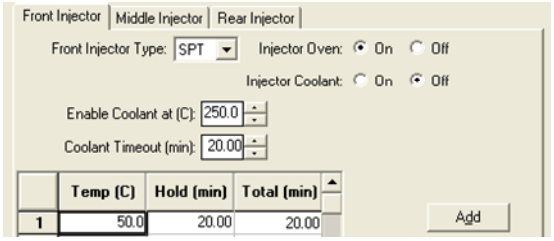
1061 Injector

Selecte the installed 1061, turn it on, and set the temperature.



SPT Injection Device

Select the desired Enable Coolant at temperature and Coolant Timeout. Create a temperature program.



Flow/Pressure Window

Flow/Pressure can have up to three EFC Programs (Front, Middle, Rear). Use the EFC Programs to specify the pressure ramp of the Type 21 or Type 25 EFC, the flow ramp of the Type 23 EFC, and the pressure ramp and total flow time program of the Type 24 EFC.

Select the type of EFC (Type 21, Type 23, Type 24, or Type 25) at each position, or select None.

Type 21 EFC and Type 25 EFC (for 1079/1177 Injectors)

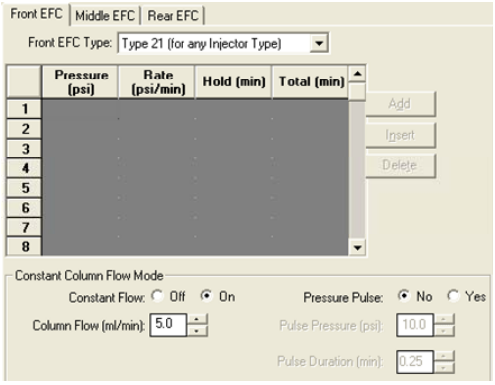
Create a pressure ramp program to control the Type 21 or Type 25 EFC.

The first row has the Initial Pressure and Hold Time for the Type 21 or Type 25 EFC. The EFC equilibrates to this setting when the method is activated, and is restored to this setting when each run is completed.

The following rows have 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. (Rate, in the first row, is always blank and cannot be edited. Also the Total column cannot be edited.)

Constant Column Flow for Type 21 or Type 25 EFC

Constant Column Flow mode is enabled in the Flow/Pressure window.



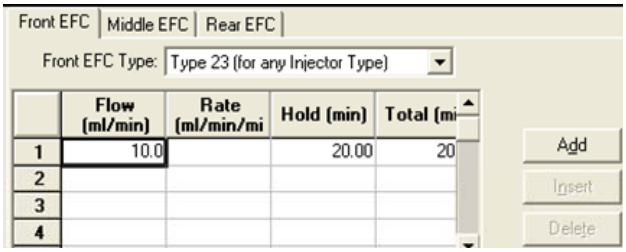
In the Constant Column Flow Mode area, click On to turn on Constant Flow. This disables the spreadsheet and shows the constant flow rate value. Type the desired Column Flow (ml/min).

When the method is activated in System Control, Workstation generates and 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 at the 450-GC front panel, and the Barometric Pressure is measured by the 450-GC at

the time 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.

Type 23 EFC (for 1041/1061 Injectors)

If a Type 23 EFC is installed and selected, a flow ramp spreadsheet is displayed.

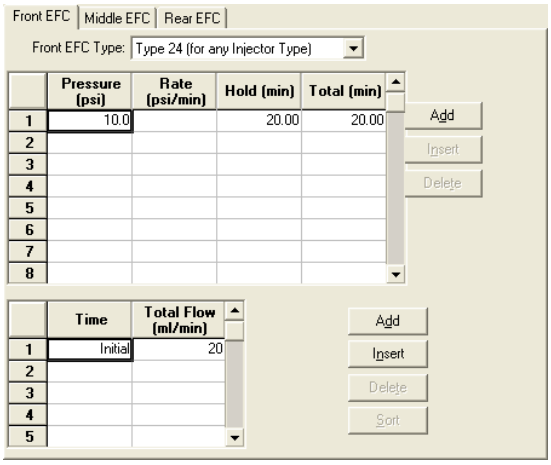


The first row has the Initial Flow and Hold Time for the Type 23 EFC. The EFC equilibrates to this setting when the method is activated, and is restored to this setting when each run is completed.

The following rows have the programmed settings for each of the ramp segments. Each segment ramps to the specified flow at the specified rate (assuming the rate is achievable), and then hold the flow for the specified time. (Rate, in the first row, is always blank and cannot be edited. Also the Total column cannot be edited.)

Type 24 EFC (for Valved Systems)

If you install a Type 24 EFC, a pressure ramp spreadsheet and a flow time program spreadsheet is displayed. The top spreadsheet is for pressure, and the bottom spreadsheet is for flow.



The first row has the Initial Pressure and Hold Time for the Type 24 EFC. The EFC equilibrates to this setting when the method is activated, and is restored to this setting when each run is completed.

The following rows have the programmed settings for each of the ramp segments. Each segment will ramp to the specified pressure at the specified rate (assuming the rate is achievable), and then hold the pressure for the specified

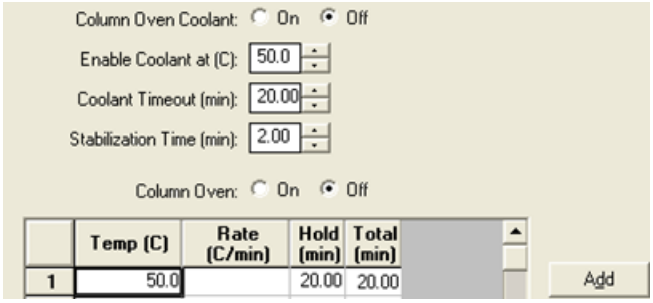
time. (Rate, in the first row, is always blank and cannot be edited. The Total column cannot be edited.)

Create flow time program to control the Type 24 EFC total flow. The first row contains the Initial Total Flow for the Type 24 EFC. The EFC equilibrates to this setting when the method is activated, and is restored to this setting when the chromatographic run is completed. The following rows after have the programmed settings for Total Flow.

Column Oven Window

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

Use the spreadsheet to build a temperature ramp program to heat and/or cool the Column Oven. Specify the desired temperature for the coolant. Specify the desired Coolant Timeout and the desired Stabilization Time.



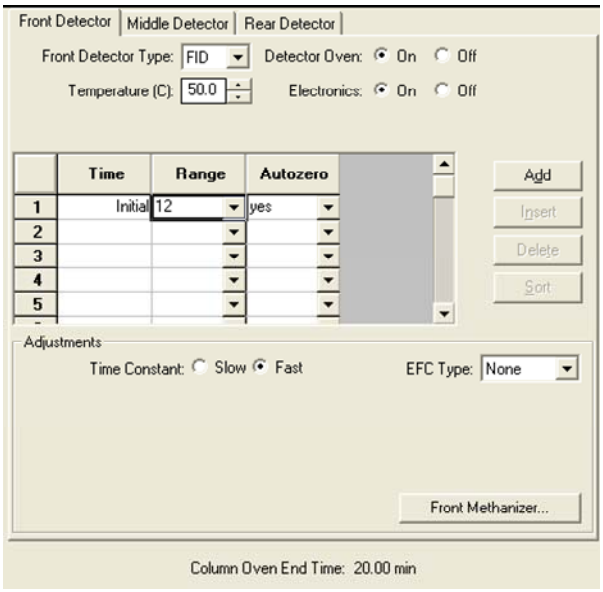
The first row has the Initial Temperature and Hold Time for the Column Oven. The Column Oven equilibrates to this setting, and stabilize for the specified Stabilization Time, when the method is activated, and is restored to this setting when each run is completed.

The following rows have the programmed settings for each ramp segment. Rate, in the first row, is always blank and cannot be edited. Also the Total column cannot be edited.

Detector Window

The Detector window has up to three Detector Programs (Front, Middle, Rear). Use the Detector Programs to specify the operating temperatures, gas flow rates and parameters of the detectors.

Use the tabs to select the Detector Program to edit. Select the type of Detector (FID, TSD, TCD, ECD, or PFPD) at each position, or select None.



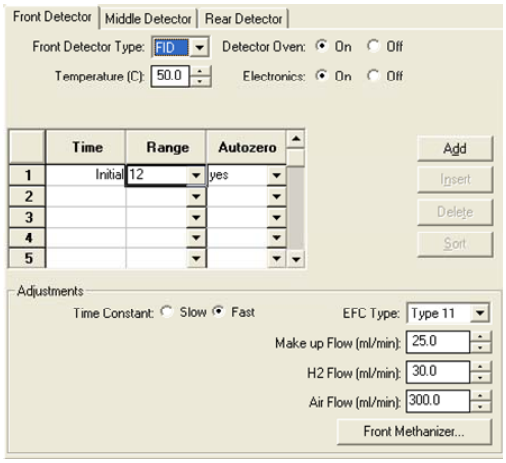
Detector EFC Modules

The detector Electronic Flow Control modules (EFC), are detector-specific and can be programmed from the Detector window. Select the type of Detector EFC at each position, or select None. Use the detector EFC program in each detector window (Front, Middle, Rear) to specify the gas flow rates for each module.

NOTE: Select the make-up gas and the auto-calibration of the module from the Detector EFC Setup and configuration screens on the 450-GC.

FID Detector

If an FID Detector is installed, an Oven Power switch, an Electronics switch, a Temperature setting and a Time Constant setting are displayed.



If you turn an FID Detector on, select the desired Temperature setting.

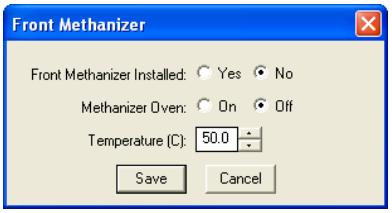
Program the Detector Range and Autozero. Select the desired FID Time Constant and select the desired gas flow rates for the detector EFC.

The first row has the Initial Range and Autozero for the FID Detector. The FID switches to this setting when the method is activated, and is restored to this setting when each run is completed.

The following rows have the programmed settings for the Range and Autozero.

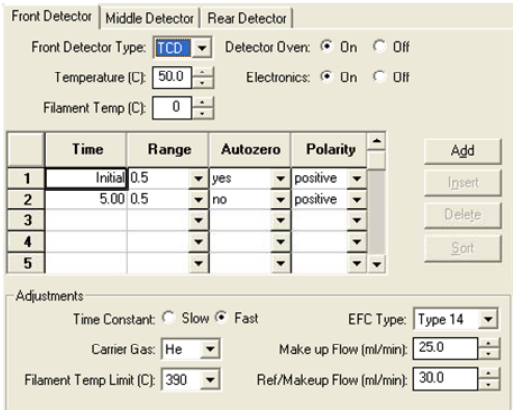
Methanizer

The Methanizer is programmed from the Detector window. Program the Methanizer in the Detector window by clicking the Methanizer button.



TCD Detector

If a TCD Detector is installed, an Oven Power switch, an Electronics switch, a Temperature setting, and a Filament Temperature setting and additional detector adjustments are displayed.



Turn on a TCD Detector and heat it by selecting the desired Temperature and Filament Temperature setting. To use the installed TCD Detector, click Detector Oven On. Program the Detector Range, Autozero, and Polarity values.

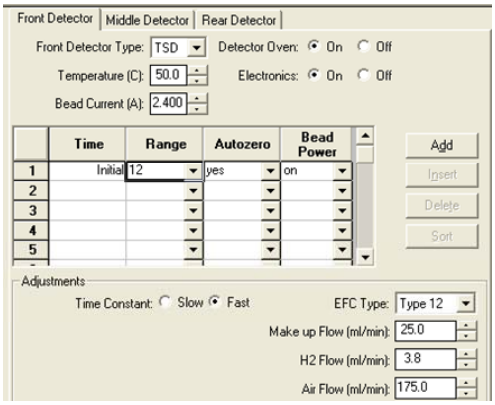
Select the desired TCD Time Constant by clicking Slow or Fast. Select the desired Carrier Gas and Filament Temperature Limit. Three EFC types are available. Select the desired gas flow rates for the sample side and the reference side of the TCD.

The first row has the Initial Range, Autozero, and Polarity for the TCD Detector. The TCD switches to this setting when the method is activated, and is restored to this setting when each run is completed.

The following row has the settings for the Range, Autozero, and Polarity.

TSD Detector

If a TSD Detector is installed switches for the following are displayed; Oven Power, Electronics, Temperature, Bead Current and Time Constant.



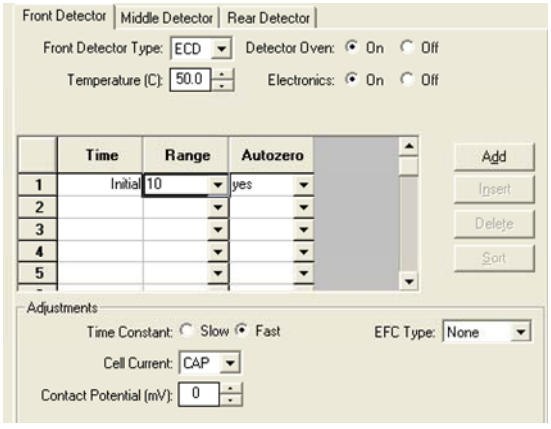
If a TSD Detector is to be turned on and heated, select the desired Temperature and Bead Current setting. Program the Detector Range, Autozero, and Bead Power. Select the desired TSD Time Constant by clicking Slow or Fast. Select the desired gas flow rates for the detector EFC.

The first row has the Initial Range, Autozero, and Bead Power settings for the TSD Detector. The TSD switches to this setting when the method is activated, and is restored to this setting when each run is completed.

The following rows have the programmed settings for the Range, Autozero, and Bead Power.

ECD Detector

If an ECD Detector is installed, an Oven Power switch, an Electronics switch, and a Temperature setting are displayed in the top, and additional detector adjustments are displayed.



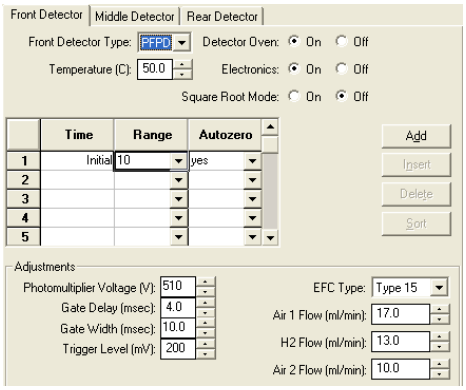
If an ECD Detector is turned on, select the desired Temperature setting. Program the Detector Range and Autozero. Select the desired ECD Time Constant by clicking Slow or Fast. Select the desired Cell Current and Contact Potential.

The first row has the Initial Range and Autozero for the ECD Detector. The ECD switches to this setting when the method is activated, and is restored to this setting when each run is completed.

The following rows have settings for the Range and Autozero.

PFPD Detector

If a PFPD Detector is installed, an Oven Power switch, an Electronics switch, Square Root Mode switch, and a Temperature setting are displayed in the top and additional detector adjustments are displayed below the spreadsheet.

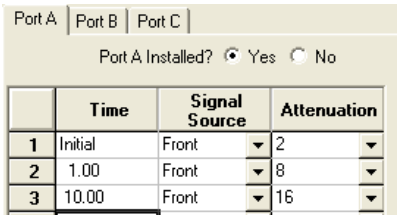


If a PFPD Detector is to be heated, select the desired Temperature setting. Program the Detector Range and Autozero. Select the desired PFPD Photomultiplier Voltage, Gate Delay, Gate Width, and Trigger. Select the desired gas flow rates.

The first row of the spreadsheet contains the Initial Range and Autozero for the PFPD Detector. The PFPD switches to this setting when the method is activated, and is restored to this setting when each run is completed.

Output Window

The Output window has up to three Output Port Programs. Use the Output Port Programs to program the Detector Signal Source and Attenuation.



Indicate if the Port is installed. Program the detector signal source and attenuation in the spreadsheet.

The first row of the spreadsheet contains the Initial Signal Source and Attenuation for the Port. The Port switches to this setting when the method is activated, and is restored to this setting when each run is completed.

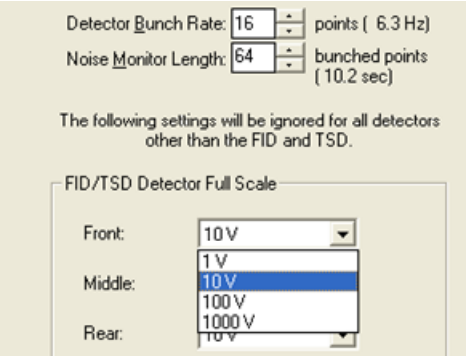
The following rows have the programmed settings for the Signal Source and Attenuation.

Data Acquisition Window

Use Data Acquisition to collect a baseline noise sample (Noise Monitor) and to select the full scale for the FID and TSD detectors. Workstation samples the baseline noise on the first derivative of the detector signal before each run. This sample is used to estimate the baseline noise. The estimate is more accurate as the sample size is increased, but the sample takes longer to acquire.

Workstation sets the full scale for the detector signal. The dynamic range of the FID and TSD detectors are equivalent to 1000V full scale, but if the peaks fall below this value, limit the full scale value.

Since Standard Report uses the attenuation setting to scale the chromatogram, the printout is based on the full scale value, use a lower full scale value to scale smaller peaks with greater resolution.



Reduce the 450-GC's 40 Hz data rate by bunching. The resulting bunched data rate is displayed to the right. Enter the size of the noise sample as the number of bunched data points. Select the full scale signal setting for the FID and TSD detectors.

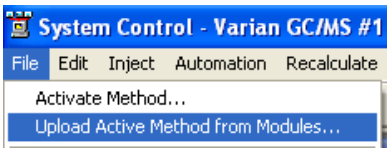
Auto-Configuring to Match the 450-GC

When a 450-GC method is edited, with the GC online in System Control, a Method Editor dialog box opens 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 as is. If you click Yes to auto-configure the Method, this dialog is displayed:

Uploading the Method from the 450-GC

Take the method from the GC and save it in MS Workstation. This permits you to do local method editing on the 450-GC front panel and then save it for later use on the Workstation.



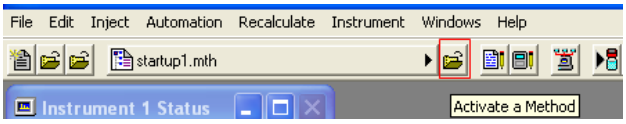
To upload the Method from the 450-GC to System Control, click File menu and then click Upload Active Method from Modules.

You are prompted for the name of the file in which to save the Method. The active Method in System Control is updated to reflect the parameters.

The Startup Method

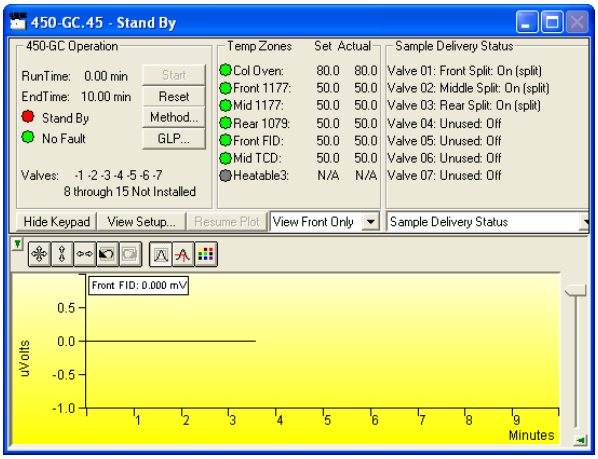
When you start System Control and display an Instrument Window, the last active Method for that instrument is activated. When System Control is started, it returns to the initial settings in the Method that was last used on the instrument.

To change Methods, simply click on the Activate a Method button on the System Control Toolbar or choose Activate Method from the File menu.



Editing Methods from 450-GC Status and Control

The 450-GC Status and Control Window has a Method button. Use it to edit the active GC Method.

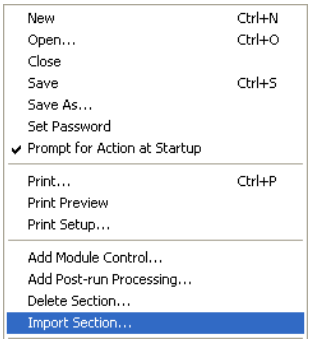


TheMethod Builder opens with active Method loaded and the corresponding Instrument Module selected. Edit that section or other sections.

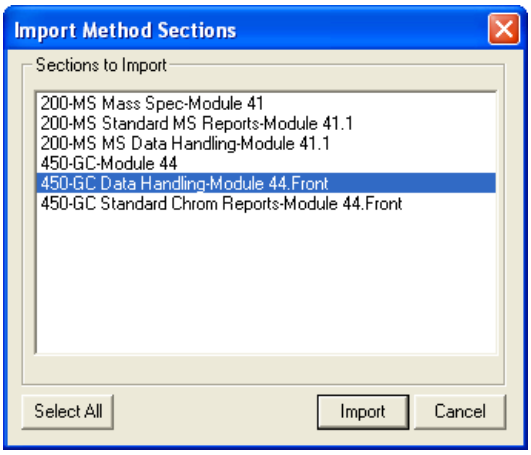
After editing the Method and closing the Method Builder window, you are prompted to reactivate the Method. Reactivating the Method downloads the changes to the Module.

Importing Method Sections

Copy sections from one 450-GC Method file to another. Open the Method file edit in Method Builder. From the Method Builder File menu, click Import Section.



Select the file with the sections to import and a dialog opens.

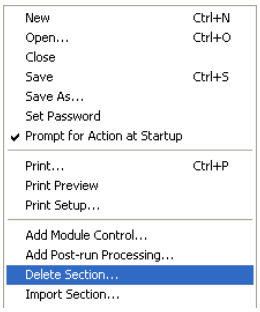


Click the sections to import. If you click on one section and the hold down the shift key while clicking on another section, all of the sections in between are selected. Holding down the control key while clicking on a section adds that selection to the files already selected. Clicking on a highlighted section while holding down the control key removes that section from the list of selected files.

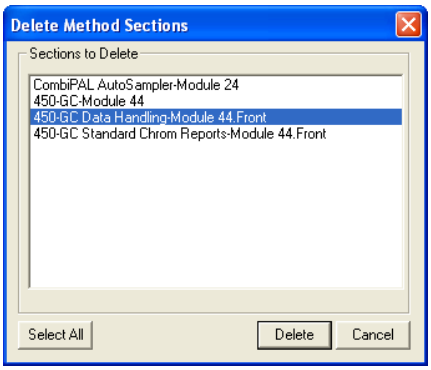
After highlighting the desired sections, click Import to import them into the Method being edited. If the Method already has sections with the same module address and channel ID, you are prompted to reassign a new module address and channel number to the imported section or overwrite the existing section in the current method.

Deleting Method Sections

To remove sections from a 450-GC method, open the method with the sections to remove in Method Builder. Click Delete Section on the Method Builder Toolbar or click Delete Section from the File menu.



A dialog box of sections contained in the Method file opens.



Select the sections you want to delete. If you click one section and the hold down the shift key while clicking on another section, all of the sections in between are selected. Holding down the control key while clicking on a section adds that selection to the files already selected. Clicking a highlighted section while holding down the control key removes that section from the list of selected files.

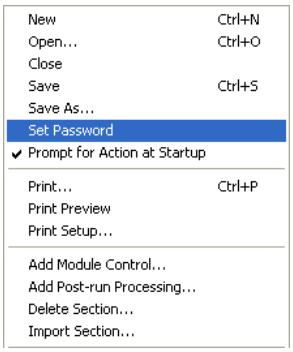
After selecting the desired sections, click Delete button to delete them from the Method being edited. You are prompted to confirm each deletion.

Printing a Method

To print a method from Method Builder, click the Print button on the Toolbar and select the Method section or sections to be printed. The active Method can also be printed from the System Control Toolbar and the MS Workstation Toolbar. Click on the Active Method Options button on the System Control Toolbar or on the Method Operations button on the MS Workstation Toolbar and select Print Method.

Password Protecting a Method

A method can be password protected from changes by clicking the Set Password button on the Method Builder Toolbar or selecting Set Password from the File menu.



Enter the password and then re-enter it to verify it.

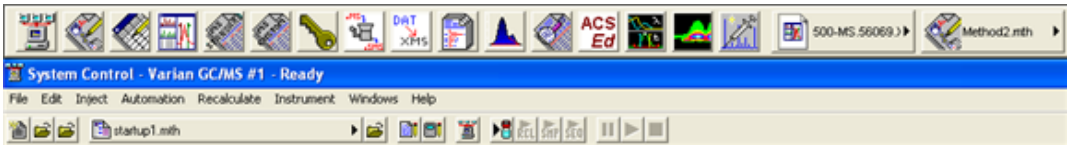
After a Method is password protected, the password is required to save changes.

After a Method is password protected, it can be activated and used for instrument control and data acquisition. It can also be viewed from Method Builder. Changes to the method cannot be saved, without using the password.

Using 431-GC Methods

Overview

Edit methods using Method Builder.



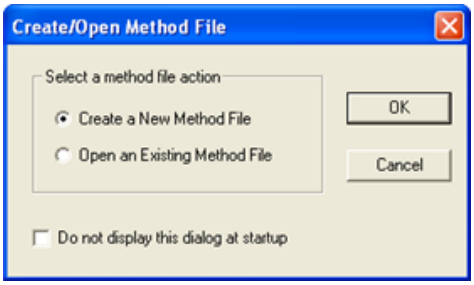
Opens Method Builder. Create a new method or open and existing one.

View and edit the method file displayed.

View and edit the method file displayed.

Using Method Builder to Create a New Method

Click Method Builder on the MS Workstation Toolbar to open the following.

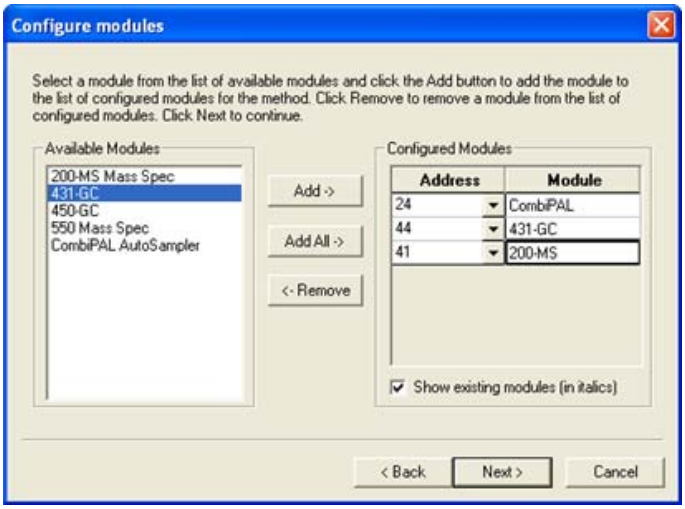


Click **Create a New Method File**, and Method Builder guides you.

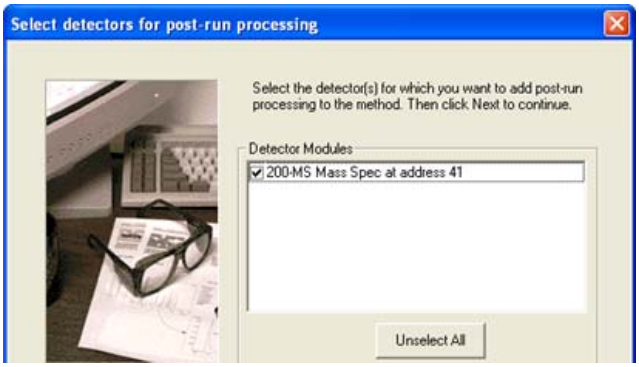
Select the instrument configuration for the method.

Click **Custom** to create a Method for an instrument not attached to Workstation.

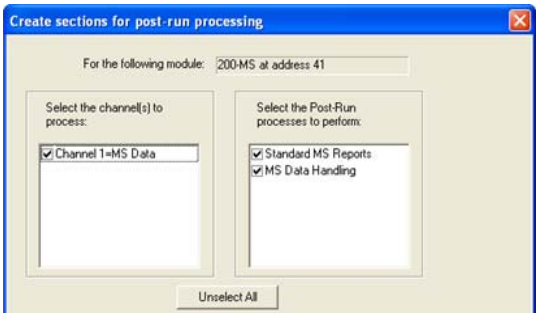
Select the modules for the method.



Select the detectors for post-run processing.



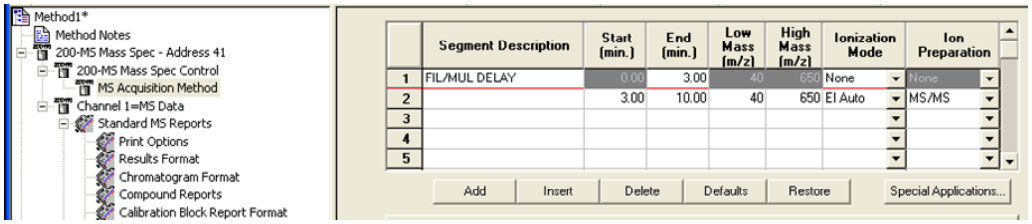
For each detector in the Method, select the channels for post-run processing.



After selecting the data channels and type(s) of post-run processing Method Builder creates a Method with the sections needed to control the hardware, collect data and do the post-run processing. These Method sections contain default values for the parameters. Edit these parameters for your analysis.

The Method Builder Window

The tree displays the method sections. Click one to show and edit the parameters.



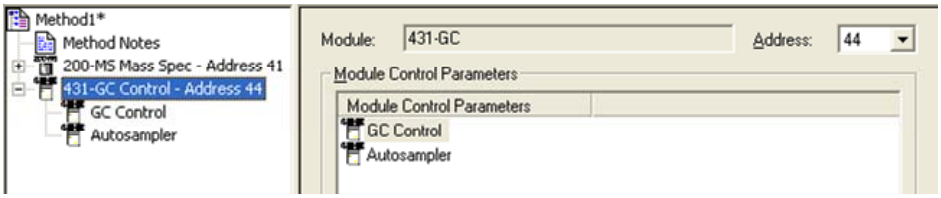
Method Notes

Method Notes, the first section, is a text field. Enter information about the Method or the application. Method Notes are displayed in the File Open dialog boxes.

Method Notes can help explain to the operator when a Method should be used. Enter sample preparation information and reminders.

The 431-GC Method Windows

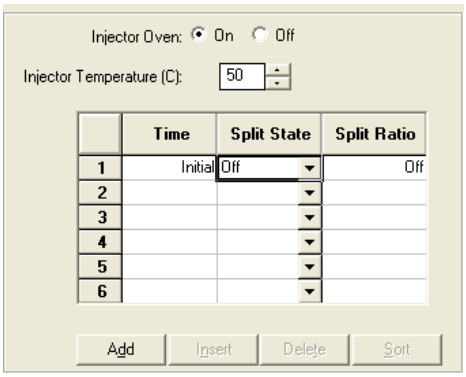
The 431-GC entry specifies the MS Workstation module address of the GC. The Address can be changed so that a Method developed for an instrument using one module address can be easily modified for use on another instrument at a different module address.



Spreadsheet Editing

Certain Method windows contain spreadsheet tables for time, temperature or flow programming. All spreadsheets behave similarly. The operations are as follows::

- Add a row at the bottom of the spreadsheet.
- Insert a row before the currently selected row.
- Delete currently selected rows and sort rows by time (available in time program spreadsheets).

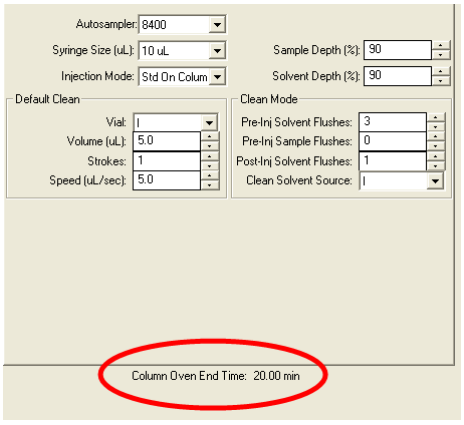


Click and drag a row numbers to select one or more rows.

Spreadsheets that specify time programs can show duplicate times, but all duplicates must be eliminated before you can save your work.

Checking Method End Times

Except for the column oven window, all editing windows show the current end time of the column oven program at the bottom.



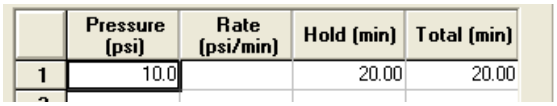
NOTE: When the Method is downloaded, component program end times exceeding the column oven end time are truncated.

GC Control Window

The GC control window contains the following sections, Flow/Pressure, Injector, and Column Oven.

Flow/Pressure

Use EFC Programs to specify the pressure ramp of the Type 21 EFC for 1177 injectors. With a Type 21 EFC installed, a pressure ramp spreadsheet opens Use it to build a pressure ramp program.



	Pressure (psi)	Rate (psi/min)	Hold (min)	Total (min)
1	10.0		20.00	20.00

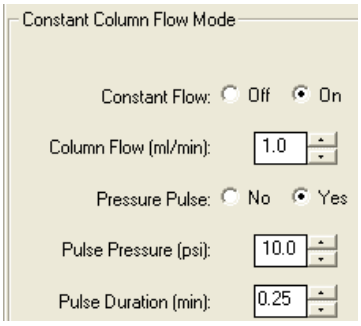
The first row has the initial pressure and hold time for the Type 21 EFC. The EFC equilibrates to this when the method is activated, and is restored to this setting after each chromatographic run.

The following rows have 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. Rate in the first row is always blank and cannot be edited and the Total column cannot be edited.

Constant Column Flow for Type 21 EFC

Enable Constant Column Flow mode in the Flow/Pressure section. Click **On** for Constant Flow to turn on the Constant Column Flow Mode. This disables the spreadsheet and shows the Constant Flow Rate value. Then, enter the desired Column Flow.

Click Yes for Pressure Pulse to perform a pressure pulse injection. After injection, the pressure changes to the Pulse Pressure for the Pulse Duration setting.



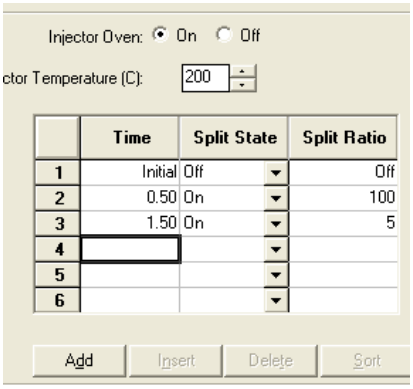
When the method is activated, Workstation generates and downloads the appropriate pressure program corresponding to the Column Temperature program, the Column Setup Length and Diameter, the Carrier Gas, and the ambient Barometric Pressure. These parameters are specified in the 431-GC System Control setup, and the the 431-GC measures barometric pressure when the Method is downloaded. The 431-GC runs the pressure program to hold the Column Flow at the specified value as the Column Temperature is ramped.

Injector Section

Use the Injector Program to set the temperature setpoints of the isothermal 1177 Injector, and split ratio of the 1177 Injector. With an 1177 Injector installed, an Oven Power switch, a Temperature setting and a Split Ratio table are displayed.

To indicate if you are using the installed 1177 injector, click On or Off for Injector Oven. Then, set the desired Temperature.

Use the Split Ratio spreadsheet to build a split ratio program to control the 1177 injector / Type 21 EFC combination. Use a split ratio of 100 after injection to vent the injector of any residual solvent. Use a very low split ratio after flushing to conserve carrier gas.



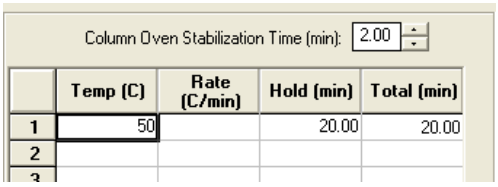
The first row has the Initial Split State and Split Ratio for the 1177 injector. The 1177 equilibrates to this setting when the method is activated, and is restored to this setting when each run is completed.

The following rows have the time-programmed settings for the 1177 Split Ratio.

Column Oven

The Column Oven window has the Column Oven Program. Use the Column Oven Program to specify the Stabilization Time of the Column Oven, and to specify its programmable temperature ramp.

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



The first row had the Initial Temperature and Hold Time for the Column Oven. The Column Oven equilibrates to this setting, and stabilizes for the specified Stabilization Time, and is restored to this setting when each run is completed.

The following rows have the programmed settings for each ramp segment. Each segment ramps to the specified temperature at the specified rate (assuming the rate is achievable), and holds the temperature for the specified time. Rate, in the first row is always blank and cannot be edited and the Total column cannot be edited.

Autosampler Window

The Autosampler window has parameters for the 8400/8410 Autosampler. Select the sampling Syringe Size, the penetration depth for sample and solvent wash Vials (Sample and Solvent Depth), the Default Clean and Clean Modes, and the Injection Modes.

Injection Mode

The Injection Mode has five predefined settings: Standard Split/Splitless, Standard On-Column, Neat, Viscous and Volatile. If any of these modes cannot satisfy your injection needs, use tge User Defined mode. Select User Defined mode to access all 8400 autosampler parameters to fine-tune your injection.

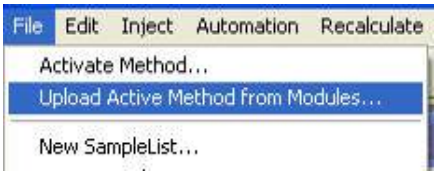
Auto-Configuring to Match the 431-GC

When you edit a 431-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 as is. If you click **Yes** to auto-configure the Method, this dialog is displayed:

Uploading the Method from the 431-GC

You can get the Method from the GC and save it in the Varian MS Workstation. This allows you to do local Method editing and then save this Method for later use on the Workstation.



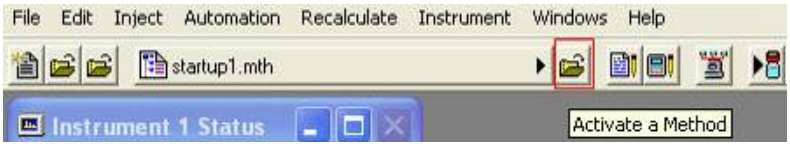
To upload the Method from the 431-GC to System Control, select Upload Active Method from Modules from the File menu.

You are then prompted for the name of the file under which to save the Method. The active Method in System Control is updated to reflect the parameters obtained from the 431-GC.

The Startup Method

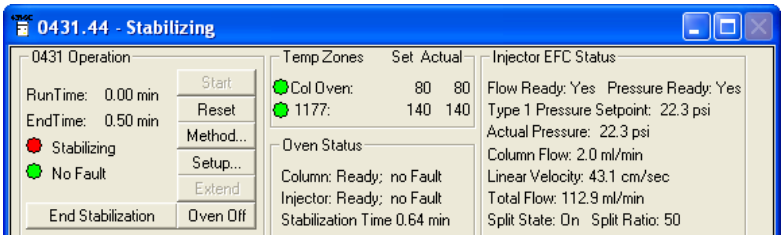
When you start System Control and display an Instrument Window, the last active Method for that instrument is activated. When System Control is started, it will return to the initial settings in the Method that was last used on the instrument.

To change Methods, simply click on the Activate a Method button on the System Control Toolbar or choose *Activate Method…* from the File menu.



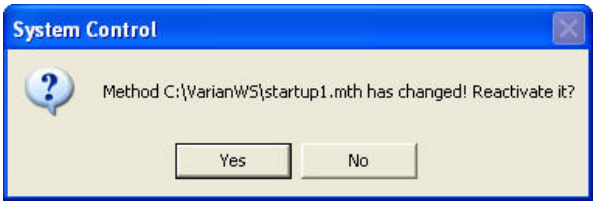
Editing Methods from 431-GC Status and Control

Click the Method button on the 431-GC Status and Control Window.



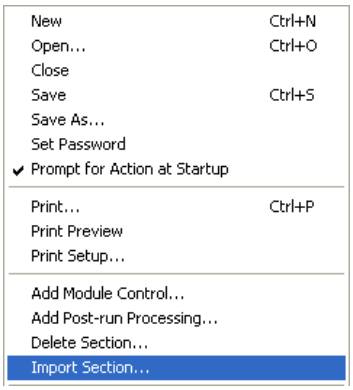
The Method Builder opens with active Method loaded and the corresponding Instrument Module selected. Edit section of the Method.

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.

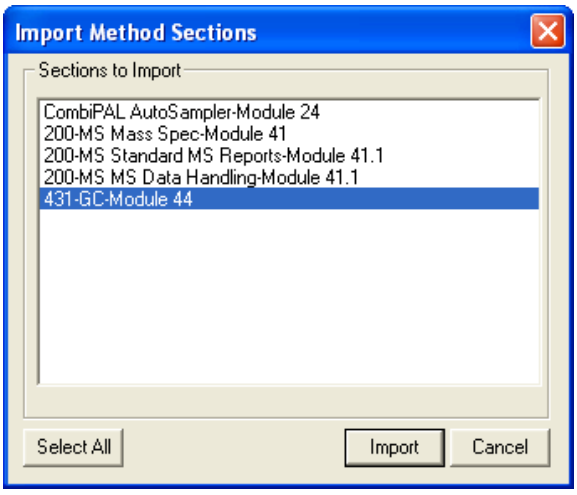


Importing Method Sections

Sections can be copied from one 431-GC Method file to another. Open the Method file to edit in Method Builder. From the Method Builder File menu, select Import Section…



Select the file containing the sections to be import. After selecting the file, a dialog box of sections in the Method is displayed.

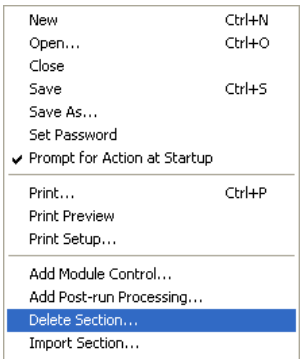


Select the sections to import. If you click on one section and the hold down the shift key while clicking on another section, all sections in between are selected. Holding down the control key while clicking on a section adds that selection to selected files. Click a highlighted section while holding down the control key removes that section from the list.

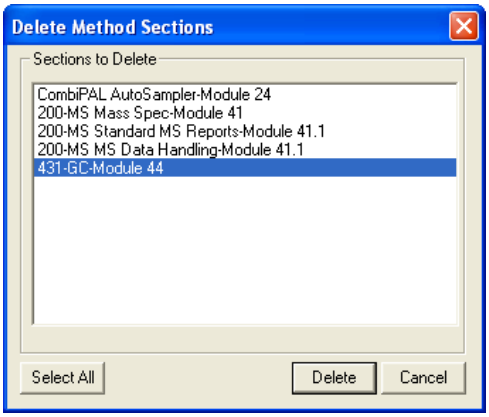
Aftere the desired sections are selected, click Import. If the Method already has sections with the same module address and channel ID, you will be prompted to reassign a new module address and channel number to the imported section or overwrite the existing section in the current method.

Deleting Method Sections

To remove sections from a 431-GC Method. open the Method in Method Builder. Click the Delete Section button on the Method Builder Toolbar or select Delete Section from the File menu.



A dialog box of the Method sections is displayed.



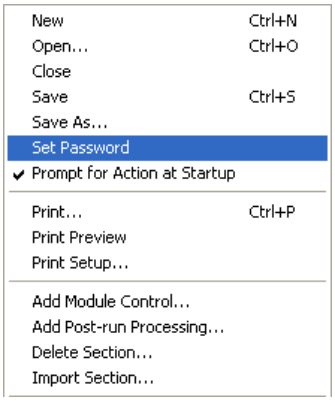
Select the sections to delete. If you click one section and the hold down the shift key while clicking on another section, all of the sections in between are selected. Holding down the control key while clicking on a section adds that selection to selected files. Click a highlighted section while holding down the control key removes that section from the list.

Printing the Method

To print a method from Method Builder, click the Print button on the Toolbar and select the section or sections to be printed. The active Method can be printed from the System Control Toolbar and the Workstation Toolbar. Click the Active Method Options button on the System Control Toolbar or on the Method Operations button on the MS Workstation Toolbar and select Print Method.

Password Protecting a Method

Password protect a method from changes by clicking Set Password on the Method Builder Toolbar or selecting Set Password from the File menu.



Enter the password and then re-enter it to verify it.

After a Method is password protected, the password is required to save changes.

After a Method is password protected, it can be activated and used for instrument control and data acquisition. It can also be viewed from Method Builder. Only the saving of changes to the Method is prevented unless the correct password is entered.

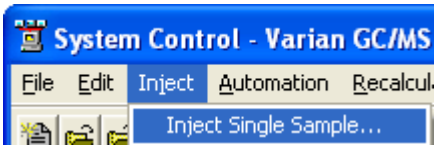
Injecting a Single Sample

Overview

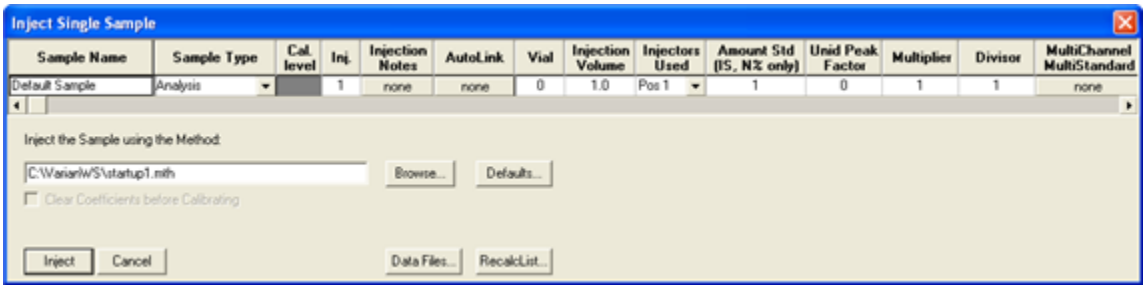
Inject a single sample with either the 450-GC or 431-GC and a Method.

Using Inject Single Sample

Inject a single sample from System Control by using the Inject Single Sample.



Display Inject Single Sample by selecting it from the Inject menu or by clicking the Inject Single Sample button on the toolbar. The Inject Single Sample dialog box is displayed.



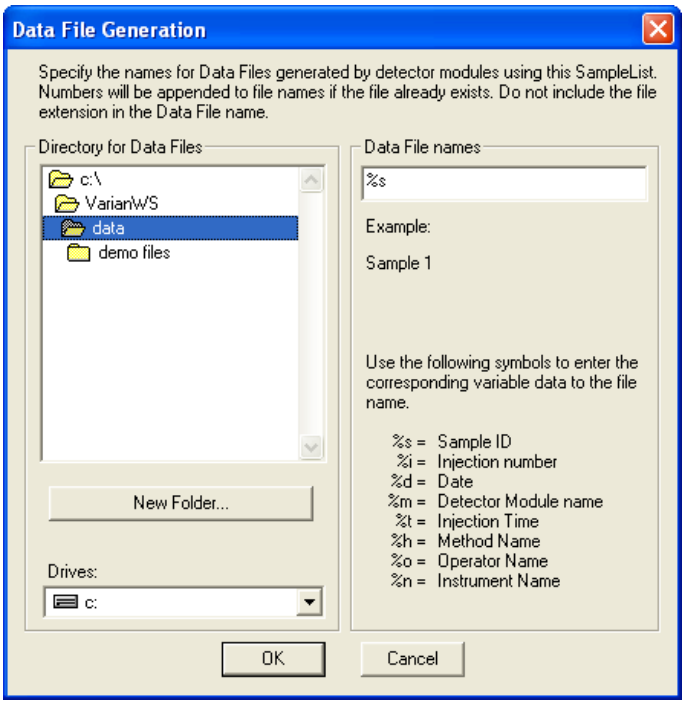
The dialog box specifies the number of injections of the sample. Enter notes about the sample. The fields in the table change depending on the type of sampling device configured in the instrument. Select the Method to use for the run and change the location and name of the Data Files. Click Inject to start the run.

If you have a 8400 AutoSampler or a 8410 AutoInjector configured, there is a shortcut. Double-click the vial position to inject from in the carousel display. This opens Inject Single Sample box with the vial number entered.

Specifying the Data File Name and Path

Data File names can be up to 255 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. When you click the Data File button, the Data Files Generation dialog box is displayed. This box the selection of the path and the filename “specification” for the data file.

Use the left side of the Data File Generation to select the drive letter and subdirectory (path) where the data files are to be stored.



Use the right to create a filename “specification”. Combine text entry with the “%” variable symbols displayed to specify filenames containing sample specific information. An example of the filename is dynamically updated as you type in the filename specification.

Specifying Per-Sample Data Handling Parameters

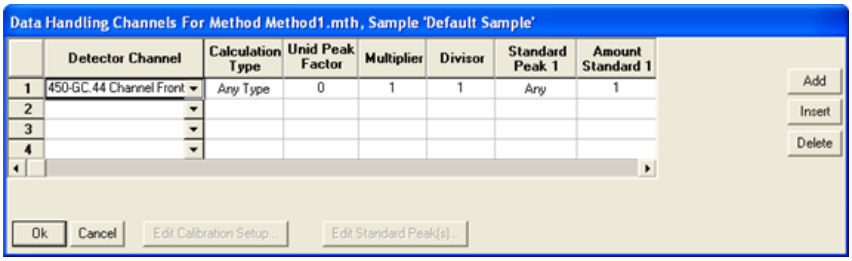
Most Data Handling parameters are specified in the Method during the injection. Some parameters may vary for each sample, and are specified when you perform the injection. The following Data Handling parameters can be specified for each sample:

- Unidentified Peak Factor
- Multiplier
- Divisor
- Amount Standard when one Internal Standard is being used

Refer to the Varian MS Workstation *Data Handling User's Guide* for a brief description. Refer to the Regulatory Compliance Manual for a complete description of how these parameters are used to calculate results.

Specify these parameters for each sample and specify them for each detector channel. This is useful if you have different detectors. In addition, if using multiple internal standards, specify their amounts for each sample and detector channel.

To access these parameters, click the button in the Multi-Channel Multi-Standard column in the Inject Single Sample box. The Data Handling Channels dialog box is displayed. When you select the detector channel in the Data Handling Channels dialog box, the calculation type and the internal standard peaks, and amounts are read from the active Method. Be sure the Method you will be using is active before you enter detector-specific parameters.



Select specific detector channels (up to 4). An amount may be entered for each internal standard peak in the Method.

Specifying a RecalcList

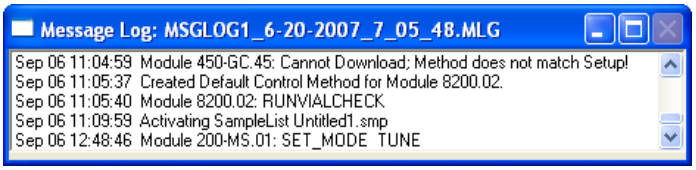
Create a new RecalcList, append to an existing RecalcList, or not create nor update a RecalcList. To select the desired RecalcList option, click the RecalcList button to open the RecalcList Generation dialog box.

A new RecalcList does not overwrite an existing RecalcList. If a RecalcList with the same filename exists, the new RecalcList has a number appended to the filename.

Monitoring the Run

After an injection is performed, monitor the status of the run in the instrument window. Module status is displayed in the status and control windows and on the toolbar. The total number of injections completed is displayed in the Instrument Status window. The list of Data Files generated in System Control, and a Quick Link button provides access to the selected file.

Automation actions and errors are recorded in the Message Log. Double-click the status bar at the bottom of System Control to display the Message Log. All Message Log entries are stamped with the time they occurred.



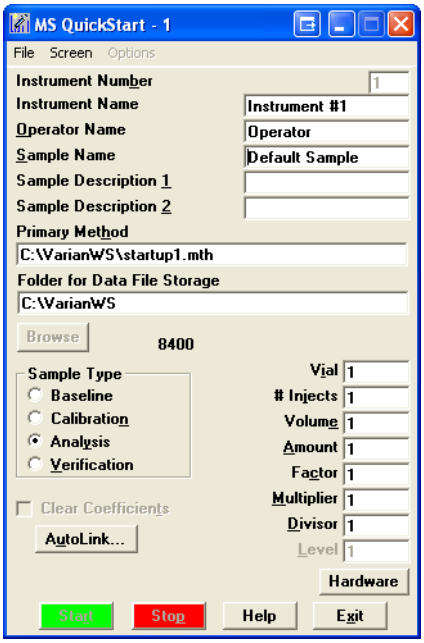
The chromatogram is displayed in the module window as it is acquired.

Using QuickStart

Use QuickStart as a fast way to inject a single sample without using System Control directly. QuickStart can be customized and is ideal for routine use. Refer to the on-line help in QuickStart for further details.

QuickStart Window

QuickStart starts System Control and waits for all modules to log in. When ready, the QuickStart window is displayed.



You can do the following in this window.

- Choose the instrument for the injection.
- Enter information about the sample.
- Enter the name of the Method you wish to use.
- Enter sampling information. This information is specific to the type of sampling device installed.
- Press Start to begin.

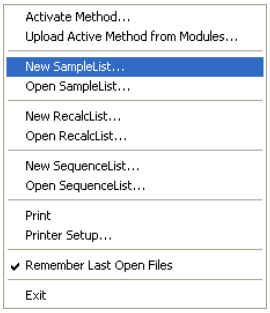
Injecting Multiple Samples

Introduction

Inject multiple samples using a SampleList using a spreadsheet to enter parameters for each sample.

Using a SampleList in System Control

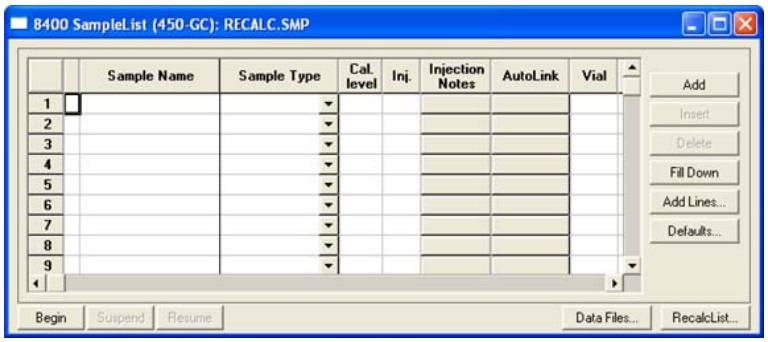
Inject multiple samples from System Control by using a SampleList. Open either a New SampleList or an existing SampleList from the File menu.



The SampleList Window

The SampleList window has fields specific to the configured sampling device. In this case, the 8400 AutoSampler is configured, the corresponding SampleList is used.

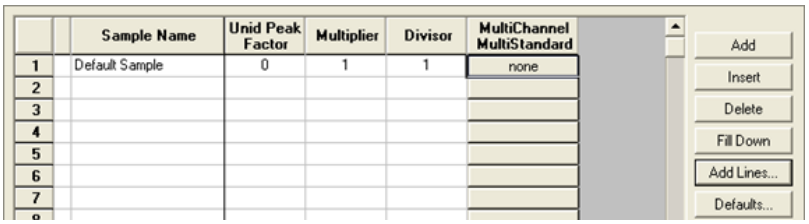
When the table is scrolled to the right, the Sample Name column does not scroll so you can see the name of the sample for which you are entering parameters. Enter data handling parameters, the amount for single internal standard calculations, the unidentified peak factor, a multiplier, and a divisor.



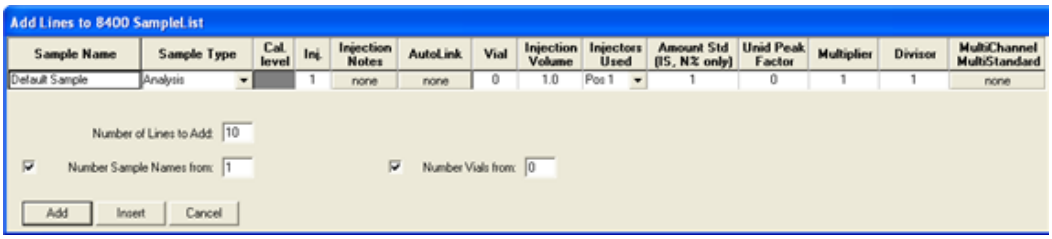
The following are the options:

- Change the size of spreadsheet columns by dragging their border with the left mouse button.
- Right-click column headers for formatting options.
- Enter notes about the sample.
- Enter post-run operations to be performed.
- Enter information about the samples and the injections.
- Select the location and name for the Data Files.
- Specify RecalcList generation options.
- Click Begin to start injecting samples.

If you have more complex requirements, such as multiple internal standards or multiple detectors requiring different entries, click the button in **MultiChannel MultiStandard** column to enter extended data handling parameters.



If you need to add several similar lines to the sample list, click Add Lines.



For sequentially numbered Sample names, enter the starting number and the number of entries to add. The Sample Names have these numbers.

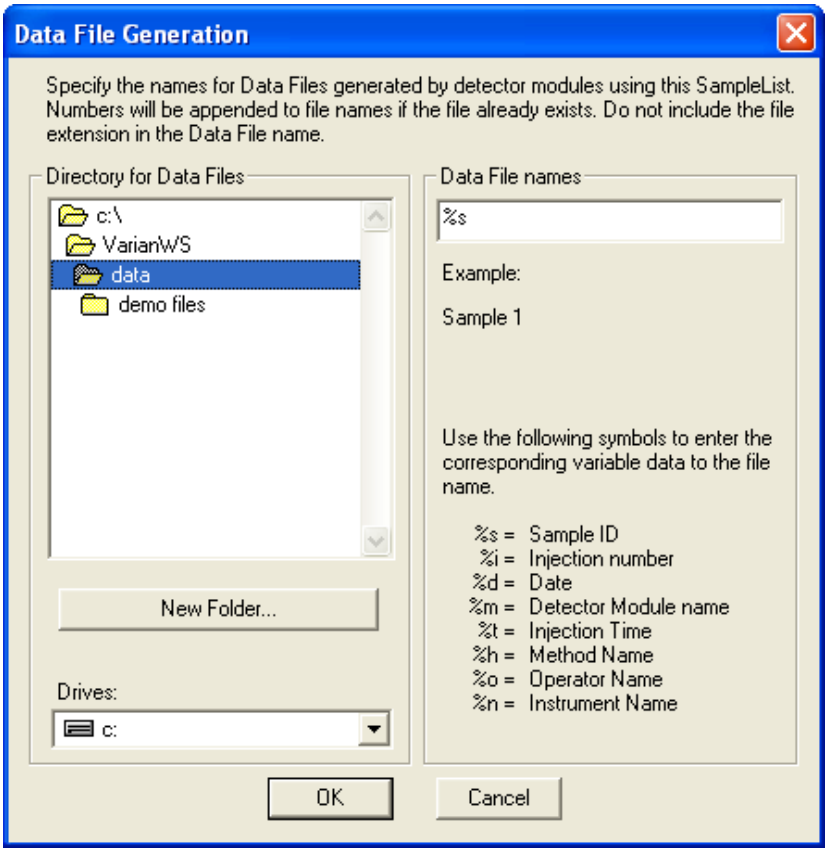
Click Begin and you are prompted for a Method. Enter the Method or browse for one.

After clicking OK, the Method is downloaded and the run begins. If you are using a manual injector or a sampling device that is not controlled by the Varian MS Workstation, start the device manually.

Specifying the Data File Name and Path

Data File names can have up to 255 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 the Data Files button to open the Data Files Generation dialog box. Select the path and the filename “specification” for the data file.

Use the left side of the Data File Generation dialog box to select the drive letter and subdirectory (path) where the data files are to be stored.



Create a filename “specification” on the right side. Combine text entry with the “%” variable symbols displayed to specify filenames that contain sample injection specific information. An example of the filename is updated as you type in the filename specification..

Specifying Per-Sample Data Handling Parameters

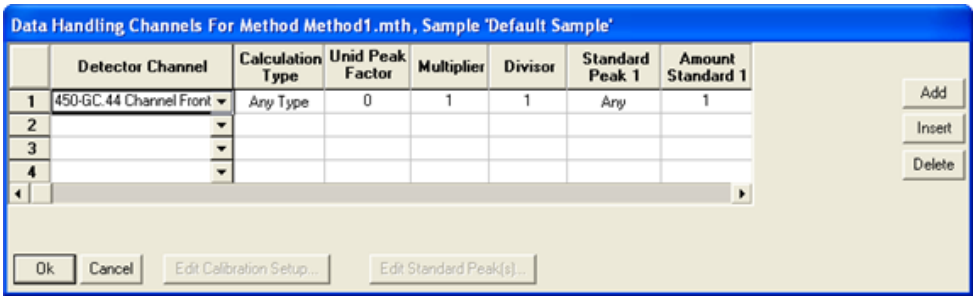
Most Data Handling parameters are specified in the Method used during the injection. Some parameters may vary for each sample, and are specified when you perform the injection. The following Data Handling parameters can be specified on a per-sample basis:

- Unidentified Peak Factor
- Multiplier
- Divisor
- Amount Standard when one Internal Standard is used

Refer to the Varian MS Workstation *Data Handling User’s Guide* for a brief description of these parameters. Refer to the Regulatory Compliance Manual for a complete description of how these parameters are used to calculate results.

Specify these parameters for each sample and for each detector channel. This is useful if you have more than one detector. In addition, if you are using multiple internal standards, specify the amounts for each sample and detector channel.

Click the button in the MultiChannel MultiStandard column in the 8400 SampleList to open the Data Handling Channels dialog box. Select the detector channel in the Data Handling Channels dialog box and the calculation type and the internal standard peaks and amounts are read from the active Method. The Method you are using is active before you enter detector-specific parameters.



Select specific detector channels (up to 4). An amount may be entered for each internal standard peak in the Method. Edit the corresponding sections of the active Method.

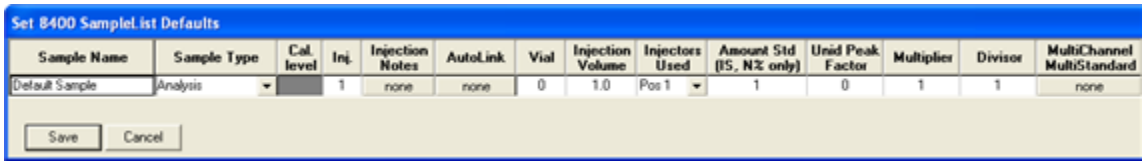
Specifying a RecalcList

Create a new RecalcList, append to an existing RecalcList, or not create nor update a RecalcList. Click the RecalcList button to open the RecalcList Generation dialog box.

A new RecalcList does not overwrite an existing RecalcList. If a RecalcList with the same filename exists, the newly RecalcList has a number appended to its filename.

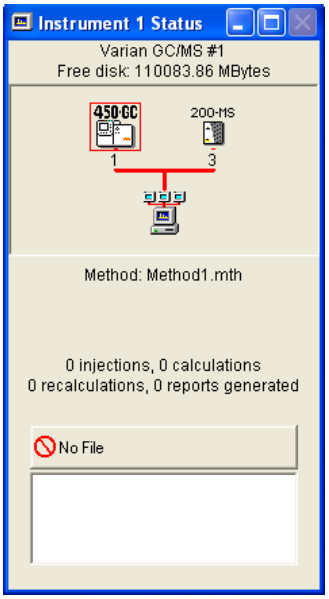
Changing Default SampleList Entries

When you add a new row into a SampleList, default values are used for each cell. To change them, click the Defaults button in the open SampleList window. Enter the desired default values and click Save.

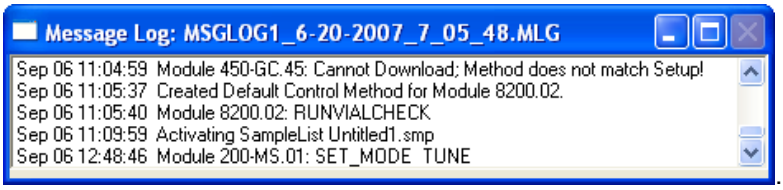


Monitoring Runs

Monitor the run in the instrument window. Module status is displayed in the status and control windows and on the toolbar. The total number of injections completed is displayed in Instrument Status. A List of Data Files generated in System Control and a Quick Link button provides access to the file.



Automation actions and errors are logged in the Message Log. Double-click the status bar at the bottom of System Control to display the Message Log. All Message Log entries are stamped with the time they occurred.



Saving SampleLists

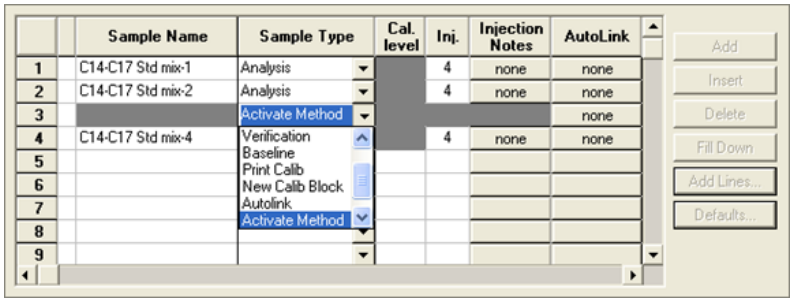
Changes made to the open SampleList, are automatically saved to the SampleList file and are used for the runs in progress. To edit a SampleList other than the open SampleList, use the offline Automation File Editor.

Using Multiple Methods for Injections

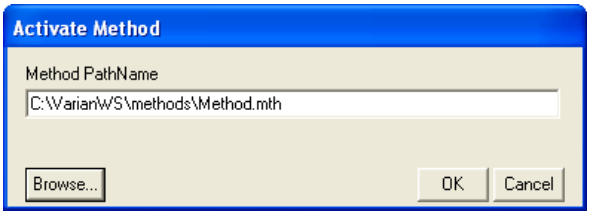
Injections can be performed injections using more than one Method. Change the active Method in the SampleList or use a Sequence.

Changing the Method in the SampleList

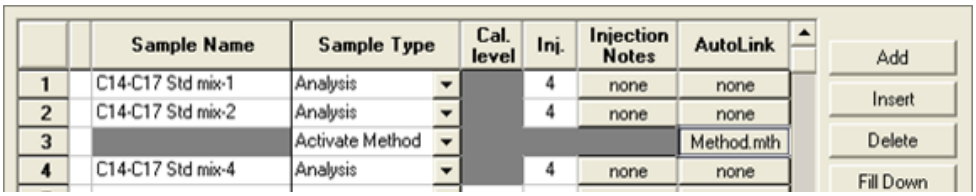
Activate a Method in a SampleList row. Select the Activate Method from the Sample Type cell. Click the AutoLink button.



Enter the Method name or pick it from the list in the Activate Method dialog box.



Specify any number of Methods in the SampleList.

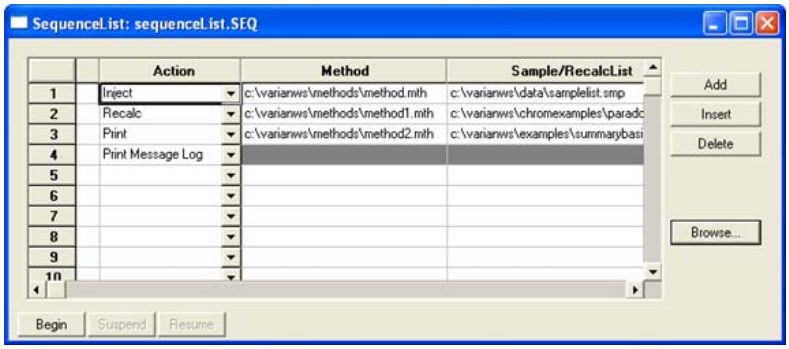


Using the Sequence Window

Use the Sequence window to specify multiple Methods and SampleLists to be processed during automation. Open a New Sequence or an existing Sequence from the System Control File menu.

The SequenceList Window

The Sequence window for the open Sequence is displayed.



You can do the following:

- Enter the Method and SampleList to use. You may enter any number of Sequence lines.
- Choose an action from the drop down box.
- Browse for a Method or SampleList file in the active cell.
- Press Begin to start the automation.

Using Automation Files

Overview

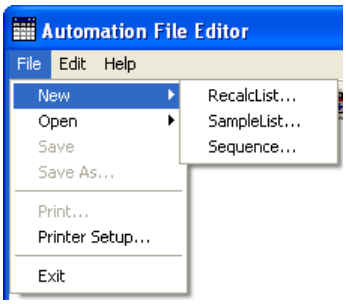
Use the Automation File Editor to edit and create SampleLists, RecalcLists, and Sequences outside of System Control. The off-line Automation File Editor allows access to files without disrupting automated runs. SampleLists and Sequences that are active and running in System Control can not be accessed in the off-line Automation File Editor.

Accessing the Automation File Editor

Click on the Automation File Editor icon on the Workstation Toolbar to open the Automation File Editor window.

Editing or Creating a RecalcList

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



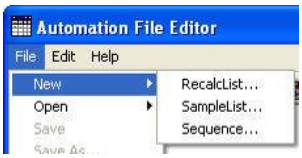
Or click the New or Open Automation File button on the toolbar.

The RecalcList window for the open RecalcList opens. It has many of the same fields as the SampleList. While the SampleList may contain AutoSampler and sample specific data handling information, the RecalcList contains the Data Filename and data file specific data handling information.

In the RecalcList window, enter post calculation operations and notes about the recalculation of the Data File. Click the reports button to view results for the selected data file. The MS Report application starts and the data file is loaded.

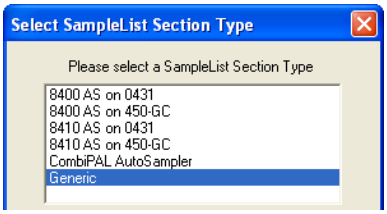
Editing or Creating a SampleList

Choose a New SampleList or Open an existing SampleList from the File menu.



Or click the New or Open Automation File button on the toolbar.

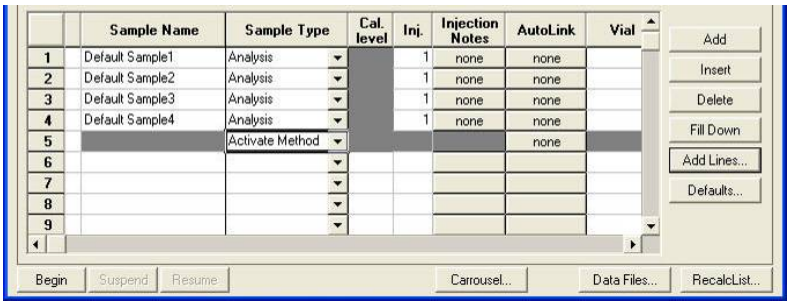
After choosing the SampleList, the “Select SampleList Section Type” dialog box opens. Choose the Generic SampleList if you are not using the 8200/SPME AutoSampler with your GC.



Change the size of spreadsheet columns by dragging their border using the left mouse button. Move columns by dragging them using the right mouse button. Right-click column headers to display formatting options.

When the table is scrolled to the right, the Sample Name column does not scroll so you can tell for which sample you are entering parameters. Data handling parameters, the amount for single internal standard calculations, the unidentified peak factor, a multiplier, and a divisor, can be entered.

NOTE: For MS data handling, the Amt Std is used as an IS Factor which is multiplied by the appropriate calibration level amount in the method.



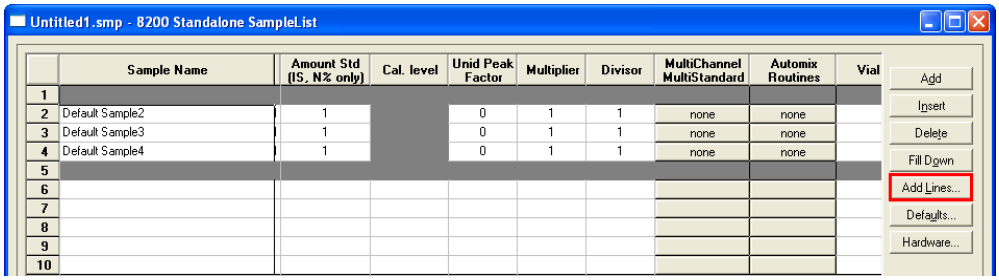
You can do the following in this window:

- Enter notes about the sample.
- Enter post-run operations to be performed.
- Enter information about the samples you plan to inject.
- Select the location and name for the Data Files.

- Specify RecalcList generation options.

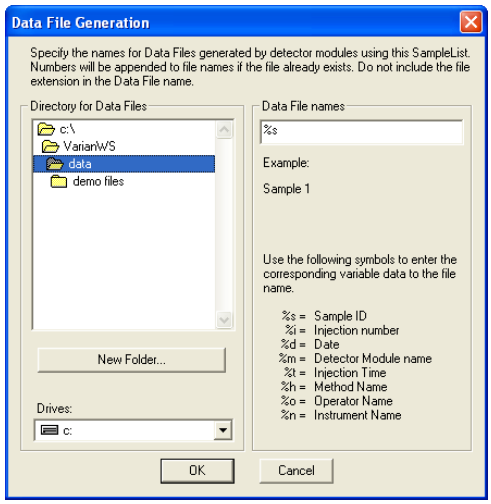
If you have more complex requirements, such as multiple internal standards or multiple detectors requiring different entries for these data handling parameters, click the button in MultiChannel MultiStandard column. For MS data handling, the specifications are contained in the method.

If you need to add several similar lines to the sample list, click the Add Lines. To sequentially number Sample names, enter the starting number and the number of entries to add. The Sample Names have these numbers appended to them.



Specifying the Data File Name and Path

Data File names can be up to 255 characters long. Sample ID, injection date, module name, and injection number can be embedded in the file name. Click the Data Files to display the Data Files Generation dialog box. Select the path and the filename specification for the data file.Use the left side of the Data File Generation dialog box allows to select the drive letter and sub-directory (path) where the data files are to be stored.



Use the right side of this dialog box to create a filename “specification”. Combine text entry with the “%” variable symbols to specify filenames that contain sample injection specific information. An example is updated as you type in the filename specification.

Specifying Per-Sample Data Handling Parameters

Most Data Handling parameters are specified in the Method during the injection. Some parameters may vary for each sample. Specify the following parameters for each sample as needed:

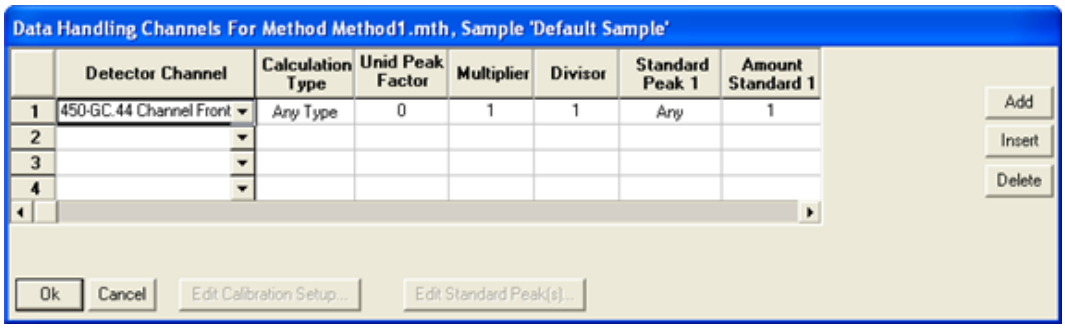
- Unidentified Peak Factor
- Multiplier
- Divisor
- Amount Standard when one Internal Standard is being used

Refer to the Varian MS Workstation *Data Handling User's Guide* for a brief description. Refer to the Regulatory Compliance Manual for a complete description of how these parameters are used to calculate results.

Specify these parameters for each sample, and for each detector channel basis. This is useful if you have different detectors. In addition, if using multiple internal standards, specify their amounts on for each sample and detector channel.

NOTE: When doing MS data handling, the specifications are made in the data handling method.

To access these Data Handling parameters, click the button in the Multi-Channel Multi-Standard column in the 8400 SampleList. You are prompted for the Method to use when this SampleList is run. Then Data Handling Channels dialog box is displayed. When you select the detector channel in the Data Handling Channels dialog box, the calculation type, internal standard peaks and amounts are read from the Method selected. The values entered for internal standard peaks and amounts are entered into the peak table of this method.



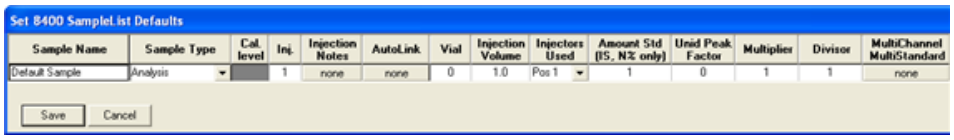
Select specific detector channels (up to 4). An amount may be entered for each internal standard peak in the Method.

Specifying a RecalcList

From the SampleList RecalcList button, create a new RecalcList, append an existing RecalcList, or not create nor update a RecalcList. New RecalcList do not overwrite existing RecalcLists. If a RecalcList with the same filename exists, the new RecalcList has number appended to its filename.

Changing Default SampleList Entries

Default values are used When a new row is added into a SampleList. To change the default values, click the Default button. The following dialog box is displayed. Enter the desired default values and click Save.



Using Multiple Methods

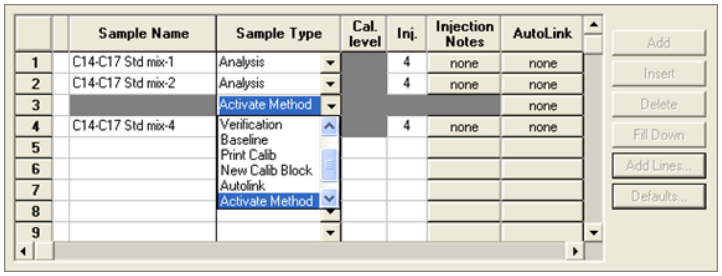
There are two ways automated injections can be performed using more than one Method.

- Change the active Method in the SampleList.
- Use a Sequence.

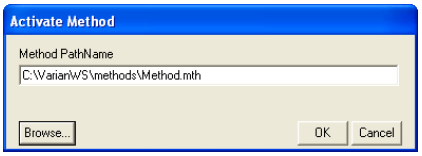
Changing the Method in the SampleList

To change the Method for injections, do the following:

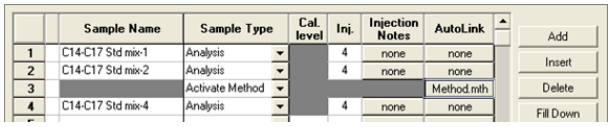
1. Activate a Method in a SampleList row.
2. Select Activate Method from the Sample Type cell.
3. Click AutoLink button.



4. Enter the name of the Method or pick the Method from a list of files.

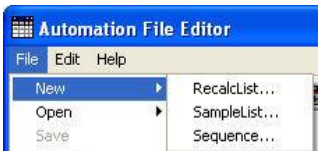


5. Specify any number of Methods in the SampleList.



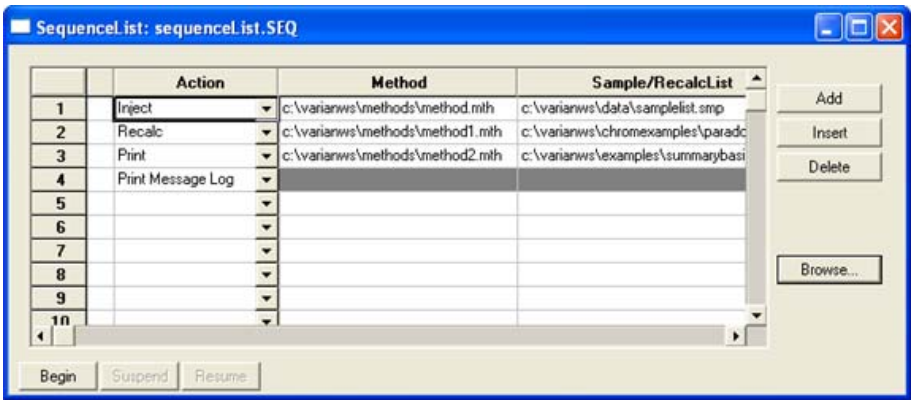
Editing or Creating a Sequence

Choose a New Sequence or Open an existing Sequence from the File menu.



Or click the New or Open Automation File button on the toolbar.

The Sequence window for the open Sequence is displayed.



You can do the following in this window:

- Enter the Method and SampleList to use. Enter any number of Sequence lines.
- Choose the action to be done in that step of the Sequence from the drop down box.
- Browse for a Method or SampleList file in the active cell.

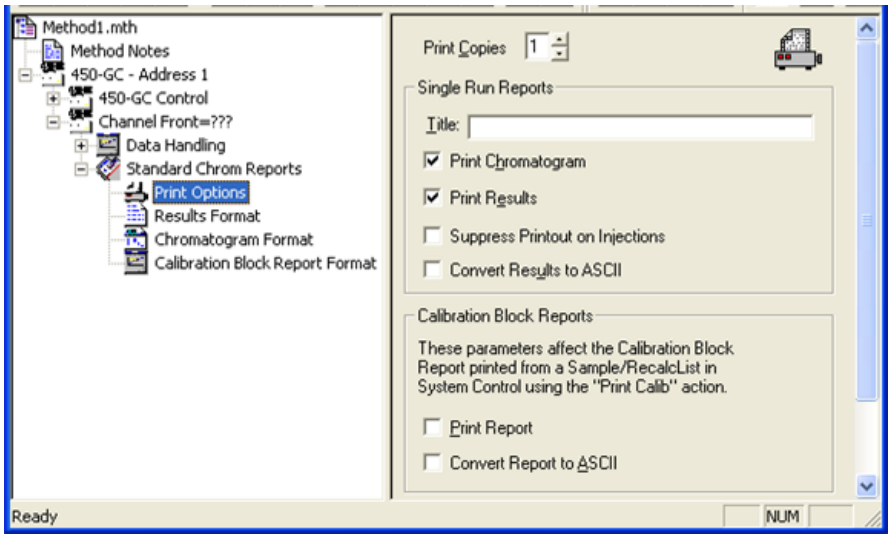
Generating GC Standard Reports

Standard GC Reports

Report formatting parameters are specified in the Report section of the Method. The Report Method section is a post-run application section for a specific detector channel. Create a Report Method section for each channel of each detector to generate a report. The section contains four editing windows.

Print Options

Use Print Options to specify the report title, if the report includes the chromatogram, results, or both, along with other parameters.

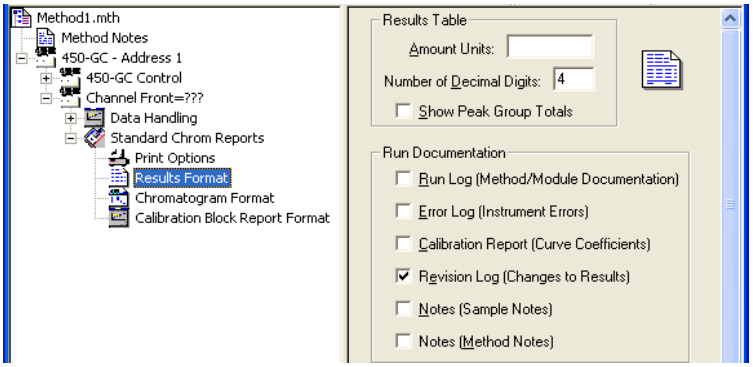


Reports print only when performing recalculations or print actions from System Control. Use Print Options to avoid automated injection delays due to printer problems.

An ASCII file can be created containing the results report. The file is named based on the Data File name and channel label, with the extension ".txt".

Results Format

Results Format specifies the layout and contents of the results report.

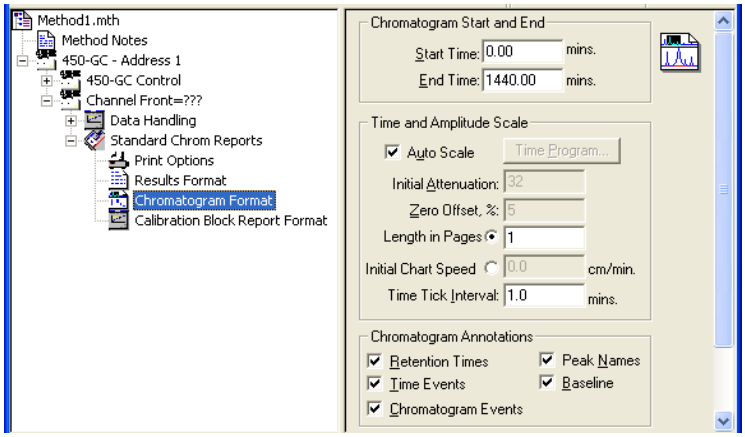


Specify any of the following from Results Format:

- Include Peak Group Totals, which uses the group number set in the Peak Table.
- Include the Method used during the injection, along with the Module Information specified in System Control.
- Include calibration coefficients and replicate statistics for each peak.
- Include date, time, and Method name logged for each recalculation of the Data File.
- Include notes entered for the Sample in the SampleList and RecalcList in System Control, or the Reintegration List in Interactive Graphics.

Chromatogram Format

Chromatogram Format specifies the length of the chromatogram, the scaling of the plot, and the plot annotations.

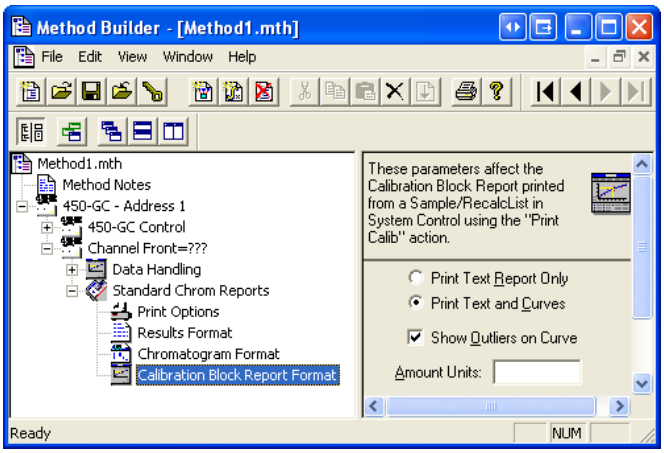


Auto Scale fits the high and low amplitudes to the page. Peaks inhibited with II or SR time events are ignored. When not using Auto Scale, click Time Program to specify attenuation and chart speed settings.

Attenuation is set in powers of two. The lowest attenuation, one, gives the most detail by making noise and other low amplitude features chromatogram easily visible. The highest attenuation, 4096, allows full-scale peaks to fit on the page.

Calibration Block Report Format

These options affect the Calibration Block Report generated when a Print Calib entry is added to a SampleList or RecalcList in System Control.

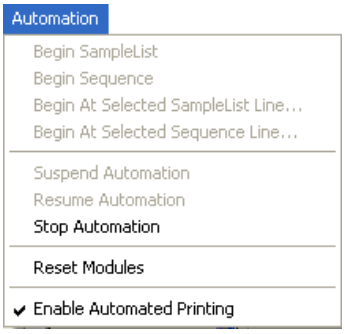


See “GC Standard Report Method Command Reference” on page 421 for more information about each window.

Automated Report Generation

After adding Report sections to the Method, generate automated reports from System Control after each injection, or after recalculations, by using the Print action in the Sequence window.

To disable automated Report printing during an automated sequence of injections or recalculations, click Disable Automated Printing from the Automation menu.

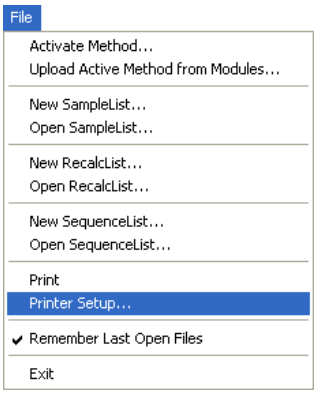


When not checked, report printing is disabled. ASCII file generation is performed, if specified in the Report Method section.

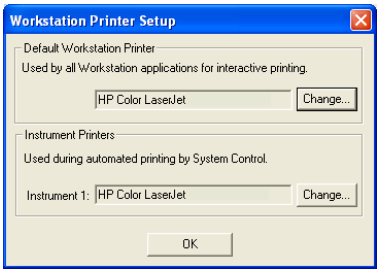
Disabling automated printing is analogous to disconnecting the printer—automation continues but no reports are printed. This is useful if you are about to run out of printer paper but do not wish to suspend automation.

Automated Printing to Multiple Printers

If running automation on more than one instrument, a separate printer can be designated for each instrument to avoid interleaving of reports. From the File menu in System Control or any Workstation application, click Printer Setup.



The Workstation Printer Setup dialog box open. This printer prints documents from any Workstation application interactively. This printer is used during automated report generation from System Control.



Batch Report Printing without Recalculating

When performing batch recalculations in System Control, reports are automatically generated using the Report parameters in the active Method. It is possible to print reports for a batch of Data Files without recalculating them.

Batch Printing in System Control

Create or open a Sequence from the File menu or toolbar. See “Using Automation Files” on page 159 for details on creating, editing, and saving RecalcLists.

Batch Printing with Batch Report

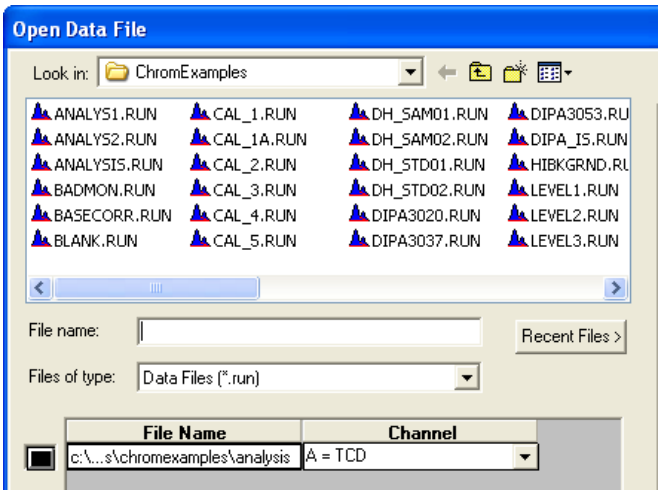
See “Using GC Batch Reports” on page 171 for more information on Batch Reports.

Viewing a Report for a Single Run

NOTE: Use other reporting applications such as the Custom MS Report Writer to view reports for Data Files.

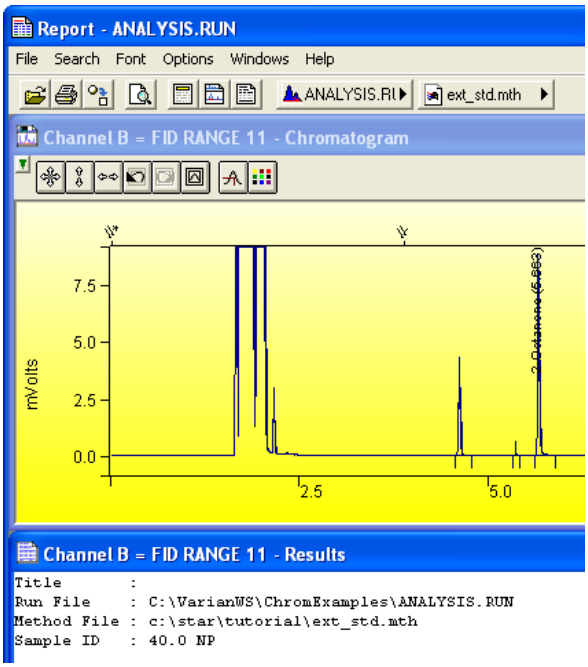
Report viewing and printing options are available from Data File Quick Link buttons, or by right-clicking on a chromatogram trace in Interactive Graphics. Select a Data File and view the chromatogram and results report by clicking the Standard GC Reports button from the MS Workstation Toolbar.

The Open Data File dialog box opens. Select the Data File, and then select the channel in the Data File to view.



The chromatogram and results report are displayed. Search for a peak name or other text in the results report using the Search menu. Specify report formatting parameters.

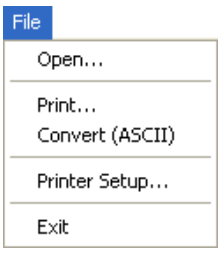
Use the Data File and Method Quick Link buttons to access additional operations, such as reintegrating the chromatogram or editing the Method.



The chromatogram is displayed with the magnification, offset and time range specified in the Report Method section most recently used on this Data File channel. The results report is displayed as it will appear when printed. When you zoom in on the chromatogram display, the chromatogram options in the Report Method section are updated.

Click the Report Title, Chromatogram Options, or Results Options buttons in the toolbar, or select the corresponding items from the Options menu, to change the report format.

From the Report application print the report, generate an ASCII of the report, or load the current Data File channel into Interactive Graphics. From the File menu print the chromatogram or the results or generate the ASCII results file.



You can also access these functions from the Report toolbar.

Using GC Batch Reports

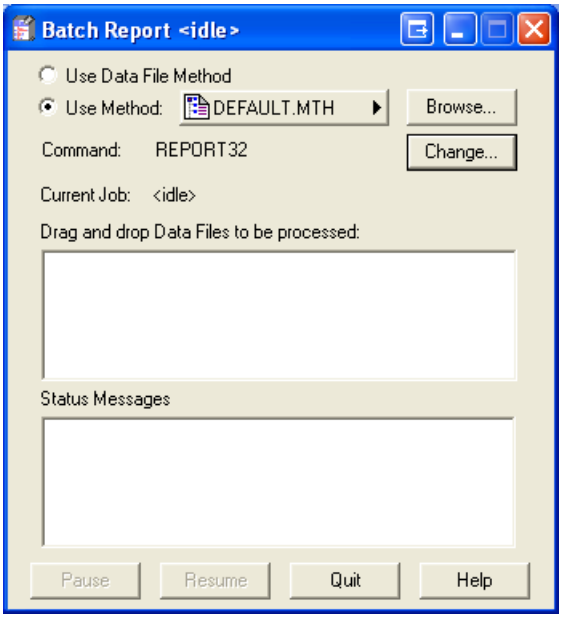
Overview

Use Batch Report to quickly generate reports for a batch of Data Files without using System Control. Reports are automatically printed when you drag and drop Data Files from the Windows Explorer onto the Batch Report window. Specify the Method to use when formatting the reports, and the post-run application.

To show the **Batch Report** window, click the **Batch Reporting** button on the MS Workstation toolbar.

Reports are printed using either the formatting options stored in the Method last used to process the Data Files or the Browse button to specify a Method. Specify the post-run application by clicking the Change button. Use REPORT32 for standard reports.

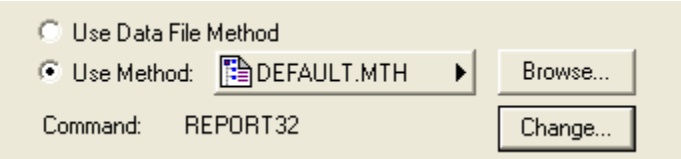
Use the Windows Explorer to drag and drop Data Files into the Batch Report window. As each report is generated, the Status Messages window is updated.



Method Selection

Use Batch Report to generate reports for a set of Data Files. Determine the Method parameters from the most recent report generation, or specify a different Method for all Data Files in the batch.

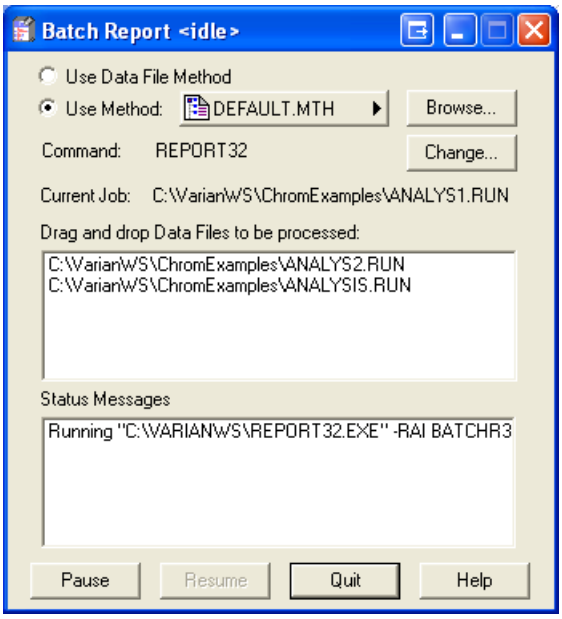
To use the Data File Method for Data File in the batch, click the **Use Data File Method** button. To use a specific Method, click the **Browse** button and then select the Method you want to use. You can view and edit the selected Method using the Quick Link button.



Generating Reports

To generate reports for Data Files using the report formatting in the specified Method, drag Data Files from Windows Explorer and then drop them on the Batch Report window. The upper list box will show the selected files. As each file is processed, a status message is added to the lower list box.

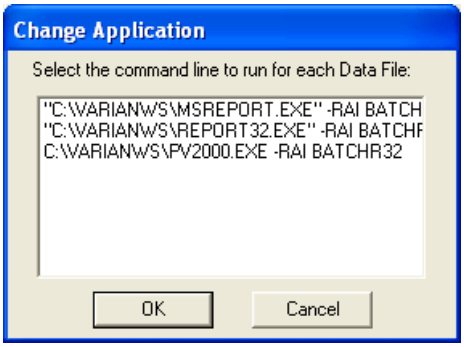
While reports are generated, click the Pause button to stop processing after the current job. When paused, the Resume button becomes available, and the batch processing can restart.



Changing Report Commands

By default, the Batch Report application generates a Standard Report for each Data File in the batch (assuming the Method contains a Standard Report section corresponding to the detector data stored in the Data File).

To select alternate report applications that were installed, click the **Change** button in the **Batch Report** window. The Change Application dialog box is displayed.



The Change Application dialog box displays all post-run applications registered in the star32.ini file in this directory: C:\VarianWS\System. The actual command line is listed for each. Select the application you wish to invoke from Batch Report and click **OK**.

Command Line	Application
REPORT32.exe	The Standard Report application.
PV2000.exe	PolyView 2000
MSREPORT32.exe	The Standard MS Report application

Calibration

Types of Calibration

Workstation has three types of calibration: External Standard, Internal Standard, and Normalized Percent. Refer to the section *GC Data Handling Fundamentals* for a brief description of each type. Refer to the Regulatory Compliance Manual for a complete description of the algorithms used by type to calculate results.

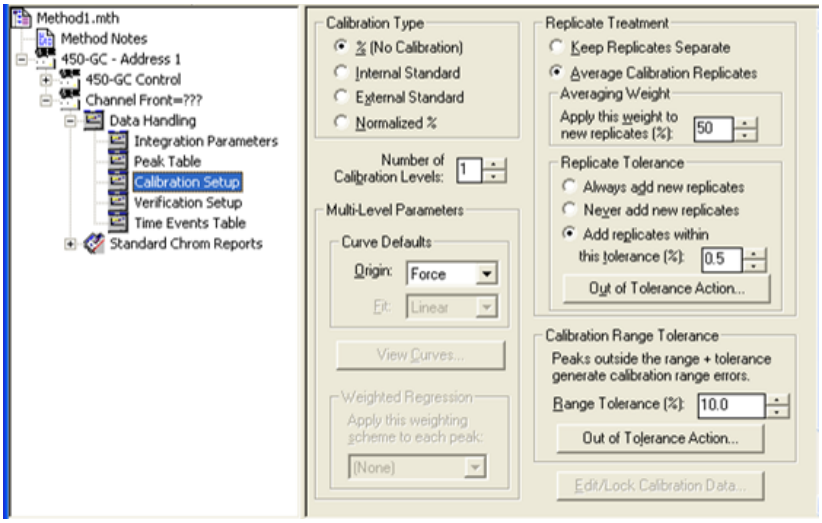
Preparing for Calibration

In order to generate quantitative results, the peaks of interest must be identified and the calibration parameters specified. Use the Peak Table and Calibration Setup window in the Data Handling section. Edit the Data Handling Method section from the Interactive Graphics or the Method Builder. Method Builder can be invoked anywhere a Method name appears in a Quick Link button.

Calibration Setup

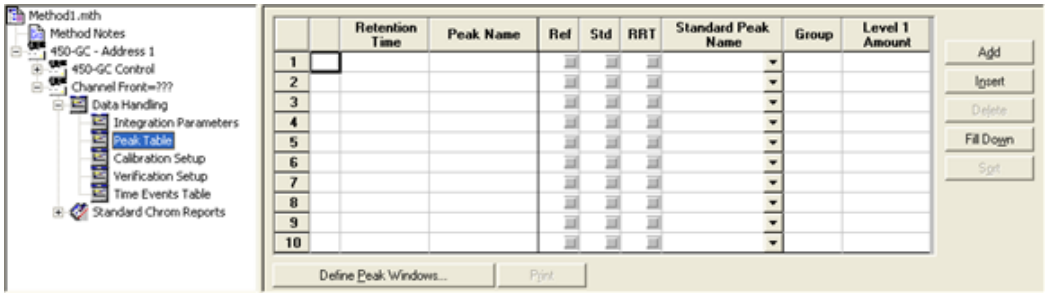
The Calibration Setup window contains parameters affecting the type of calibration calculations performed.

Specify the calibration type. Up to 10 separate replicates are allowed. The percent of new versus historical data can be obtained. See the Online Help in Interactive Graphics for a description of all fields in this window. See the Regulatory Compliance Manual for a description of weighting options.



Peak Table

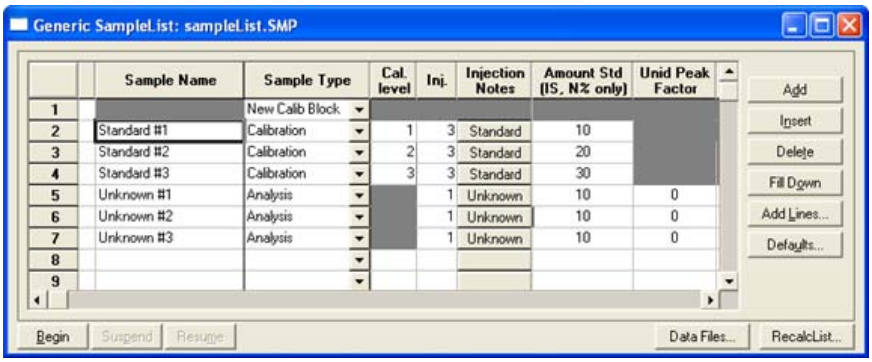
The Peak Table has amounts for each level (the number of which is specified in the Calibration Setup) and the internal standard peak. Specify internal standard peaks, refer to the appropriate standard peak, and enter amounts for each level.



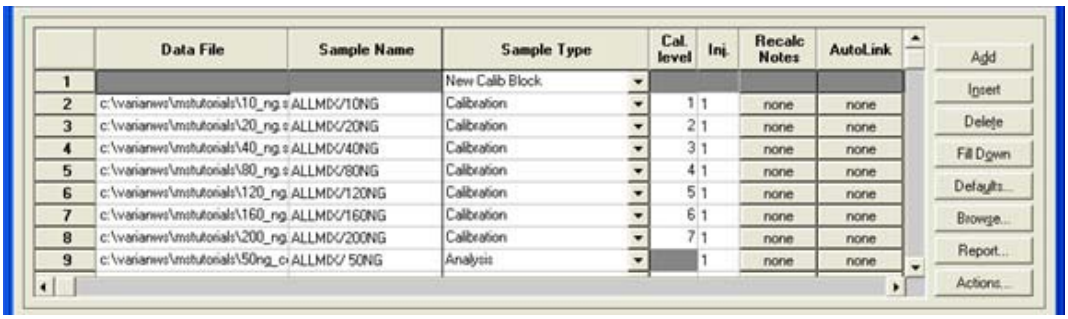
Automated Calibration

Calibrate your Method by injecting calibration samples. Calibration samples are specified in the SampleList. To clear previously stored calibration data, enter a New Calib Block line.

In the SampleList, specify the internal standard amounts, select the Calibration sample type, and enter the calibration level for this injection. Inject more than one replicate for each level.

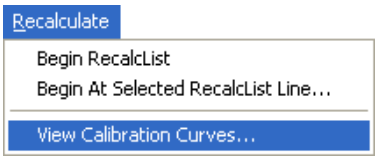


Calibrate your Method using previously collected Data Files, recalculating them as calibration samples. Add the Data Files to the RecalcList, select the calibration sample type, and enter the calibration level for this data file.

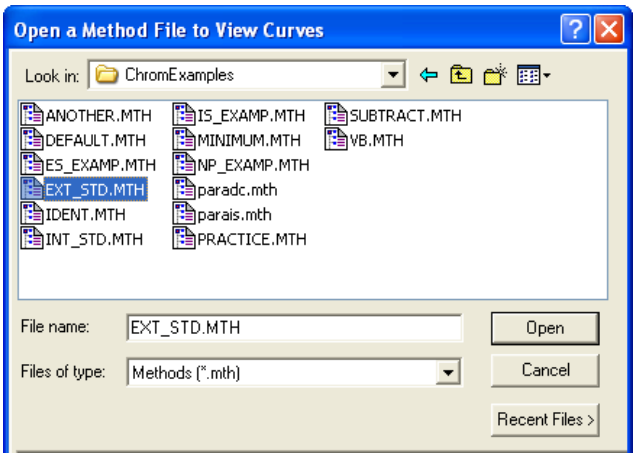


Inspecting Calibration Curves

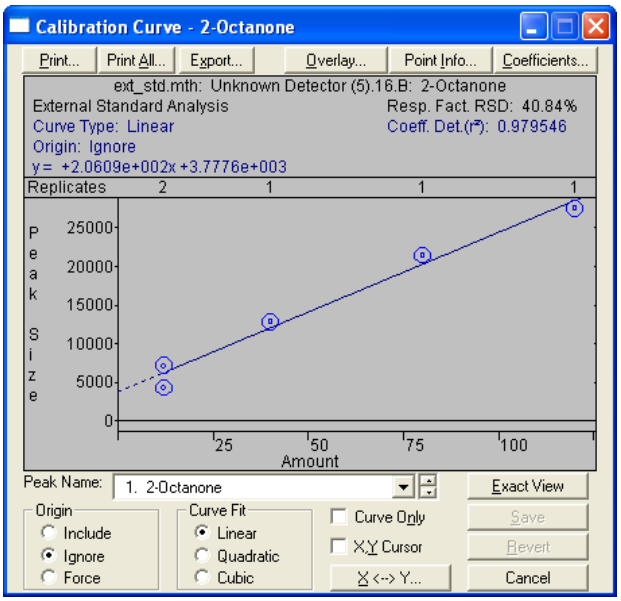
View and edit Calibration Curves from System Control. From the Recalculate menu select View Calibration Curves.



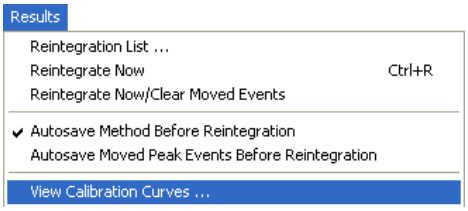
You are prompted for the Method containing the calibration curves. The active Method is selected by default.



If curves exist for more than one channel, you are prompted for the channel. The Calibration Curve window is displayed.



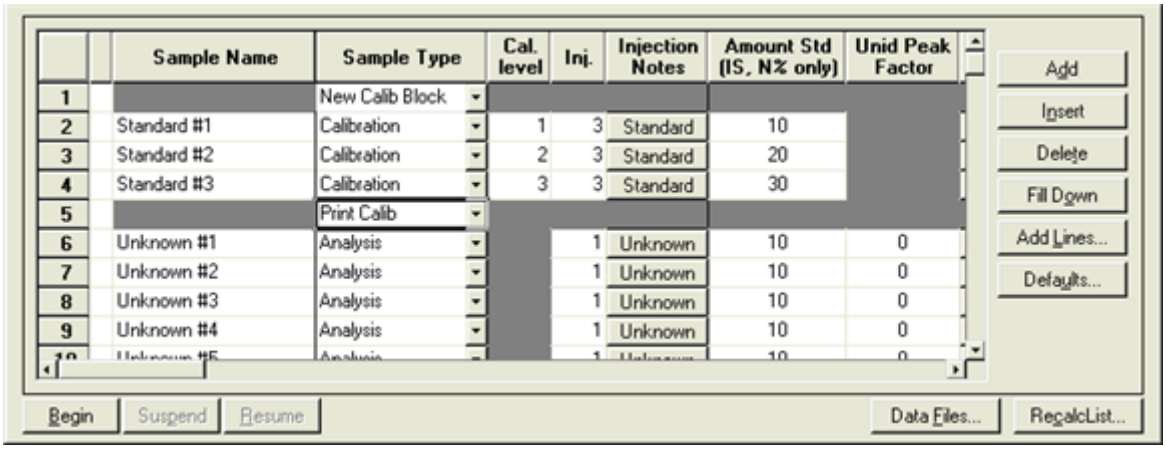
View Calibration Curves for the active Method in Interactive Graphics. From the Results menu select View Calibration Curves.



View Calibration Curves from the Calibration Setup window in the Data Handling section of the Method. Click the View Curves button.

Generating Calibration Block Reports

As calibration information in System Control is created,generate a Calibration Block Report documenting the calibration curves and replicate statistics for each peak. Open the SampleList (displayed) or RecalcList window and then enter a Print Calib line after all calibration runs are completed.

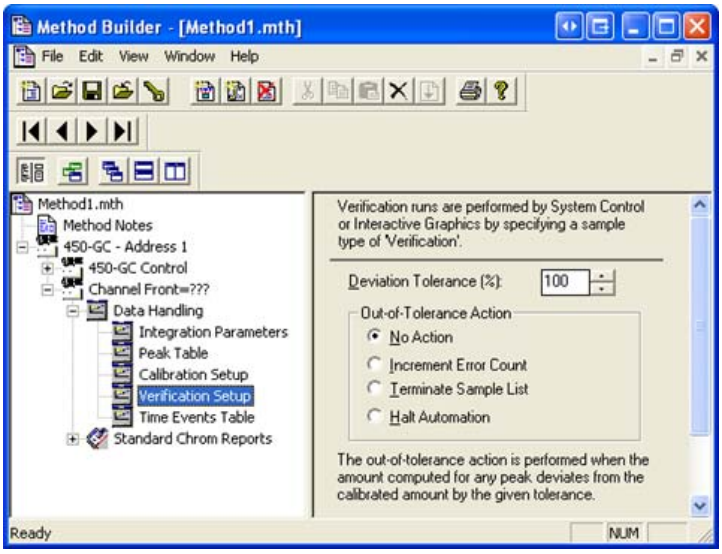


A Calibration Block Report is printed when the SampleList or RecalcList line is encountered. The format of the Calibration Block Report is determined by the Calibration Block Report Format parameters.

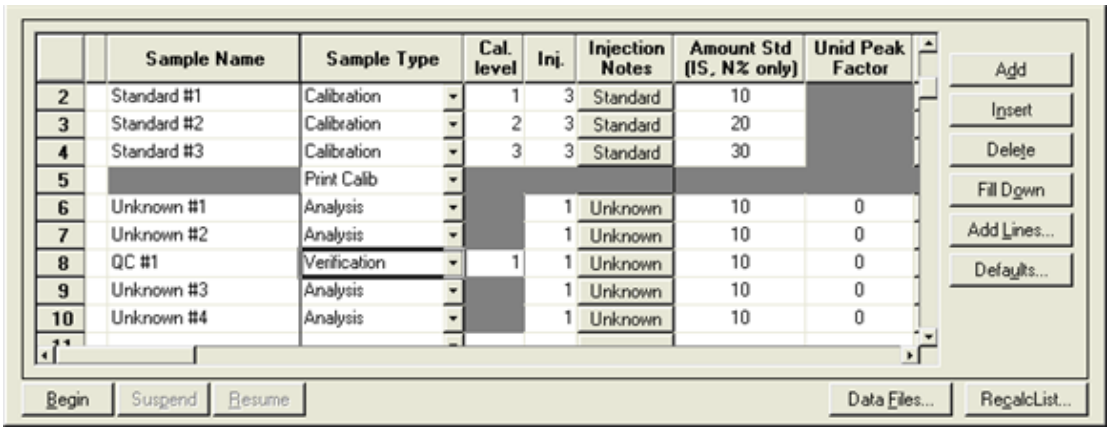
Calibration Verification

It is possible to periodically check the validity of calibration data as the injections are performed. Inject a verification sample with known amounts for each compound and compare them to amounts calculated from the calibration curves. If the amounts deviate more than a given tolerance, a verification failure occurs and a failure actions can take place.

Verification failure options are specified in the Verification Setup window in the Data Handling Method section. Type the Deviation Tolerance, and then select the failure action. Verification failures are documented in the results report.



Verification samples are entered into the SampleList (displayed) or RecalcList. In the SampleList, select Verification in the Sample Type column, and then type the calibration level corresponding to the known amounts in the sample in Cal. level.



GC Data Handling

Introduction

Unresolved peaks or other situations may require special post-run Data Handling operations. For example, excluding solvent peaks from the total area when doing area percent calculations. You may want to ensure that a very small peak in one part of the chromatogram is detected, and not rejected as a noise peak. Another use is to fine tuning quantitation method.

Refer to the *Calibration* section for more information on calibration and verification procedures. Refer to the Regulatory Compliance Manual for a complete description of Data Handling algorithms and calculations.

Performing a Pilot Run

Perform a pilot run to adjust the Data Handling parameters. Use Interactive Graphics to edit the Data Handling section of and save this with the Instrument Control sections for automatic data analysis on production runs.

Develop Data Handling Methods using an iterative approach in Interactive Graphics. Change Method parameters, reintegrate, and then determine if the results of changes are appropriate. If not, repeat these steps until you have the desired results. View the pilot run and create a Peak Table by clicking a peak of interest. Add timed integration events using the Interactive Time Events. Generate and review the calibration curves used to calculate results.

Peak Detection

Workstation uses four steps to analyze the raw data:

- Peak detection
- Peak integration (and final baseline determination)
- Peak identification (if a Peak Table is present)
- Results calculations

Peak Detection: The peak start, apex, and end points are determined. Fused peaks are identified as a precursor/tangent peak pair, or as two valley separated main peaks.The programmable time events that affect the peak detection process are Peak Width, Signal to Noise Ratio, Inhibit Integrate, Tangent Percentage, and Forced Peak.

Peak Integration: Process any Split Peak events. This causes a previously detected peak to be treated as two separate peaks. Baseline placement affects both peak detection and peak integration. The four time events which determine

baseline placement do not affect peak detection. These events are Valley Baseline, Horizontal Forward, Horizontal Backward, and Horizontal Minimum.

Optionally, identify the peaks. Exclud peaks using the Solvent Reject event or the Peak Reject event. Treat several peaks as one peak using the Group Peak event. Peaks are matched by retention time with a list of peaks previously entered in the Peak Table.

Perform the required calculations.

Peak Width Determination

Set an initial peak width parameter to acommidate potential peak width differences from run to run. The lower the peak width value, the more accurate the placement of peak events. However, if set too low, a wide short peak may not be detected.

Peaks tend to widen with incresing retention time. Use an automatically programming peak width event for different times. Early eluting narrow peaks can use a low peak width setting, while later eluting wide peaks can be detected with a higher peak width setting. The software monitors peak widths as the peaks are detected. If it determines that peaks are getting too wide relative to the current peak width setting, it programs a wider peak width. The software can automatically program narrower peak width settings.

Instead of using the software, peak width setting can be programmed manually. Manually programming a peak width event disables automatic peak width programming. In most cases, automatic peak width determination is enough.

Adjusting the Signal-to-Noise Ratio

The Signal-to-Noise Ratio (S/N ratio) affects peak detection. When the the S/N ratio is decrease, small noise peaks may be detected. Conversely, increasing the S/N ratio results in the detection of fewer small peaks. In the extreme, a high S/N ratio may not detect some peaks of interest, particularly if the manually programmed peak width value is too low. Another effect of a high S/N ratio value is that peak start and end events tend to be closer to the peak apex, especially when there is a lot of tailing, or a sloping baseline. This can result in a valley separated peaks incorrectly considered baseline resolved.

The optimal setting for this value is analysis dependant. Set this value low enough so desired peaks are detected, but high enough so extraneous noise is not detected as peaks. To detect peaks in one part of the chromatogram, but not in another, program different S/N ratio values at different times.

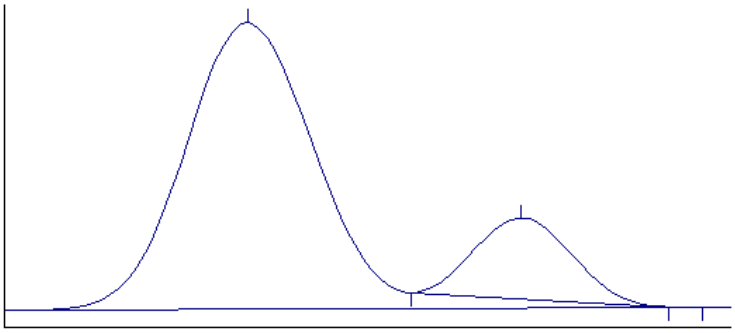
Rejecting Solvent Peaks

In many analyses, there is an unretained solvent peak at the beginning of the run. This is the solvent of your sample, and is not significant for the results. There are two options for removing the peak from the results—use the Inhibit Integrate or the Solvent Reject event. Inhibit Integrate occurs during peak detection. This event removes the specified section of the chromatogram from consideration for peak detection. With the Inhibit Integrate event, regardless of the location of the event end, the next detected peak always starts a new baseline. Use Solvent Reject if your analyte is a shoulder peak or is tangent to the solvent peak. This allows the peak detection algorithms to correctly

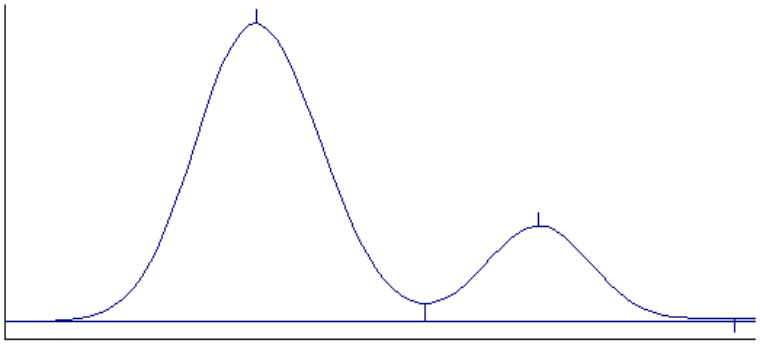
determine the baseline points for the shoulder or tangent peak, while still removing the solvent peak from the results calculations.

Skimming Fused Peaks

Fused peaks are peaks that are not baseline resolved. Peak detection treats fused peaks as valley separated peaks, as tangent peaks, or as fused tangent peaks. The Tangent Percentage value affects which peaks are considered valley separated peaks and which are tangent peaks. The Tangent Percentage value represents the percentage of the peak height of the second peak to the first. If the peak height of the second peak is a lower percentage than the Tangent Percentage, then the peak is considered a tangent, otherwise it is considered a main peak. Generally, the higher the programmed Tangent Percentage value, more peaks are considered tangents. A tangent peak can only be detected after a main peak. Tangent skimming cannot be done on leading tangents.



Tangent Skimmed Peak



Valley Separated Peaks

Fused tangent peaks are a special case of tangent peaks. After determining that more than one peak is tangent to a main peak, separate the tangents by valleys.

Splitting Fused Peaks

Occasionally, shoulder peaks are not detected, especially if there is no defined valley between the fused peaks. The area is treated as one peak, even two peaks are expected. Use the Split Peak event to split one peak into two valley separated peaks.

Forcing Peaks

Forcing peaks is a way of defining baselines. If after adjusting the S/N ratio and peak width, a desired peak is still not detected use forcing peaks. Alternatively, use the Forced Peak event to group multiple peaks so they are reported as one peak (see also the Group Peak event).

The Forced Peak event places peak events at the start and end times of the event and draws a baseline between them. The apex is the highest data point in the event time range. This event supersedes all other peak detection events, so the Peak Width, Signal to Noise Ratio, Inhibit Integrate, and Tangent Percentage settings have no effect on the forced peak placement.

Identifying Peaks

Use the Peak Table to identify Peaks. The Peak Table is in the Data Handling section of the Method. The Peak Table lists the names of compounds and their expected retention times. Since retention times may vary slightly from run to run, specify a window for identifing a particular peak. The peak window is the span of time that the software searches for the peak, centered around the retention time entered. If the peak falls within that time window, it is identified, otherwise it is not identified. While unidentified peaks can be reported, they cannot be accurately quantified (refer to the on-line help in Interactive Graphics for a description of the unidentified peak factor).

If the peaks drift, automatically modify their peak windows by marking a peak as a reference peak. Non-reference peaks have their peak windows adjusted by the same percentage that the reference peaks have deviated from their expected retention times.

Use Interactive Graphics to build a Peak Table using the pilot run. Select the Fill Peak Table from the Edit menu and click each peak in the pilot run which you want to identify. As a peak is clicked, a new entry is added to the Peak Table with the retention time and a default name. After adding all the peaks of interest, change the default names to real compound names.

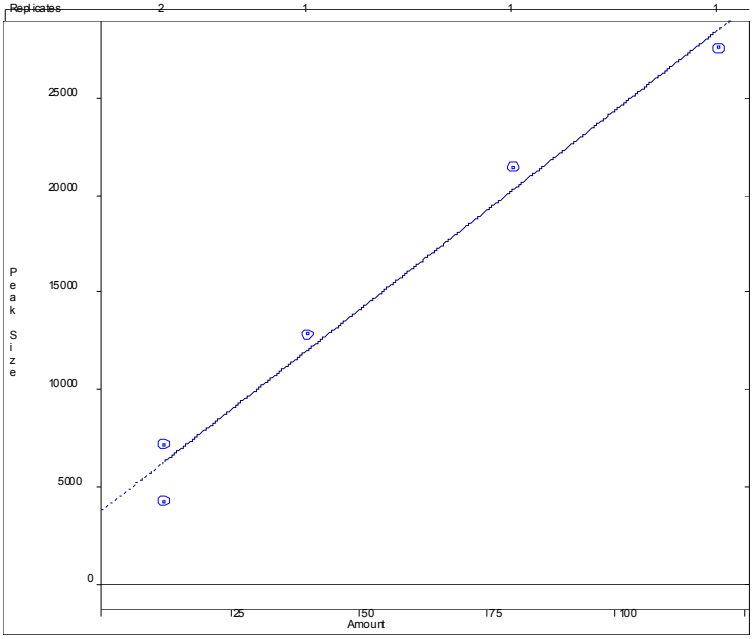
Building a Calibration Curve

The amount of an analyte is determined by comparing the peak area of a sample peak to the peak area from a sample with a known amount of the compound. Samples containg known amounts of analytes are calibration standards. Designate the run of the calibration standard as a Calibration Run. Enter amounts (for each analyte in the calibration standard) in the Peak Table.

Sometimes several calibration runs are needed, and in each successive calibration run inject different calibration standards with different amounts of each analyte. This is multipoint or multilevel calibration. MS Workstation allows calibration of up to ten levels. Each level represents the amount of each analyte for each calibration standard. Multilevel calibration can be more accurate than single level calibration because you can calibrate over large range. For more accuracy, repeat injections l to average the injection to injection variation.

The calibration curve for an analyte is generated by plotting the peak size on the y axis and the injected amount on the x axis for each calibration run, and then

calculating the best line through the points. The options area linear, quadratic or cubic fit.



Sample Calibration Curve Using Linear Fit

Designate injections of sample with unkown amounts of analytes as Analysis Runs. After identifying the desired peaks, they are quantified with the calibration curve. The peak area is the y value in the calibration curve equation. The x value is the analyte amount.

External Standard Calibration

External Standard calibration is the most common method. First perform a calibration run with a standard mixture. The calibration curve manager automatically generates a curve by plotting the known amounts of standards, as entered in the Peak Table, against the corresponding peak area. When a sample is injected in an analysis run, MS Workstation calculates the amount of the analyte.

Internal Standard Calibration

To use an Internal Standard calibration, calibrate with calibration standards containing a known amount of another analyte, the internal standard. The internal standard is also added to each sample. When making an injection, any variation in the injection volume is reflected by a detectable variation in the amount of the internal standard. The process used to prepare the samples may cause fluctuations. Adding the internal standards before sample preparation corrects for recovery. The Peak Table may contain as many as eight internal standard peaks. Each non-standard peak refers to the internal standard peak for

calculations. Using multiple internal standards allows matching each peak to a standard with similar chemical properties, which should have a similar recovery.

Ratios are plotted to generate the Internal Standard Calibration curve. The ratio is of the peak area divided by the standard peak area on the y axis and amount of standard divided by the amount of internal standard on the x axis. Even if the injection volume varies slightly, the ratio of the sample to the internal standard remains constant.

Normalized Percent Calibration

Normalize percent calibration gives a percentage amount of each analyte relative to the total amount of all analytes in the sample, adjusted for varying detector responses to the different analytes. It is analogous to a regular percentage calculation, except that the percentages are based on actual amounts of sample components rather than on peak size. It is also analogous to Internal Standard calibration in that the amounts are determined using a calibration curve based on ratios of sample to internal standard. An alternative method of generating ratios of amounts is to use Internal Standard or External Standard calibration and choose Normalize Results in the Integration Parameters.

Choosing a Calibration Type

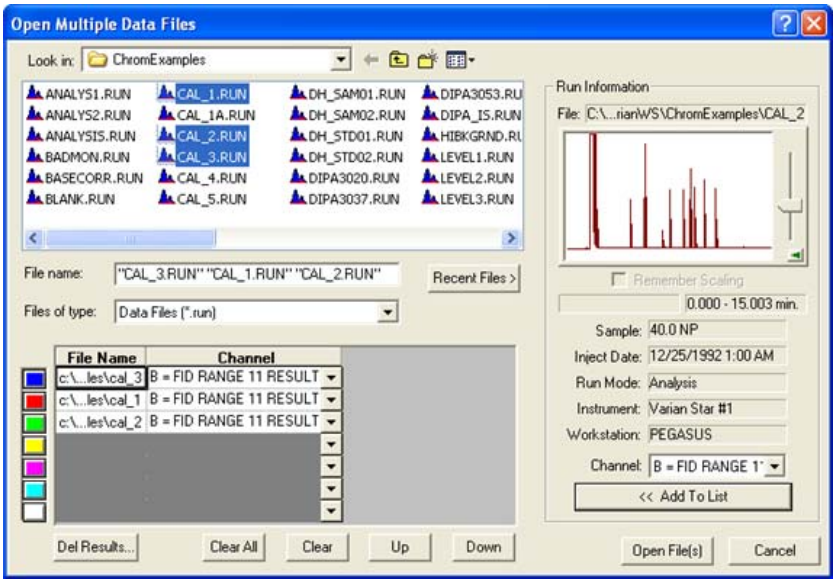
The calibration type to use depends on regulatory requirements and sample workup techniques. If you can very accurately measure your standard amounts, using an external standard calibration type is the easiest. The Internal Standard calibration type accurately accounts for variances in injection volume or if you have varying losses during sample preparation.

Using GC Interactive Graphics

Viewing Chromatograms

Use Interactive Graphics to review chromatograms, edit Data Handling Method parameters, and recalculate results. Launch Interactive Graphics from the MS Workstation Toolbar by clicking the Interactive Graphics/Data Handling button.

If the desired Data File appears in a QuickLink button, select View/Edit Chromatogram from the menu. If you did not select View/Edit Chromatogram from a QuickLink menu, you are offered up to seven Data Files to open when Interactive Graphics opens.



To select files, do one of the following:

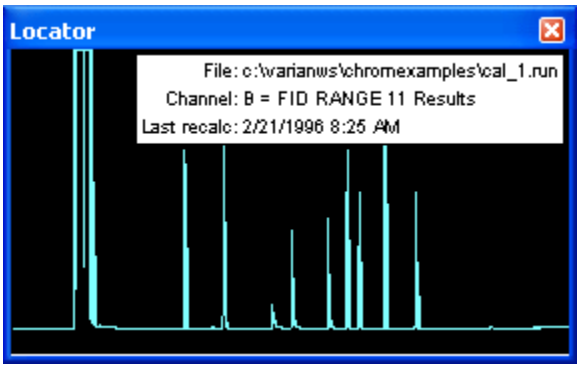
- Double-click the file name.
- Select the file name, and then click the Add To List button.
- Drag and drop the files over the list of files.

In the list of files, change the detector channel or re-order the files. When finished, click Open Files to view the files.

Interactive Graphics Window

The selected file or files are displayed in the Interactive Graphics window. The window includes a main toolbar, a chromatogram display, Visual Method Editing, Attenuation Control, and the Locator window.

The Locator Window



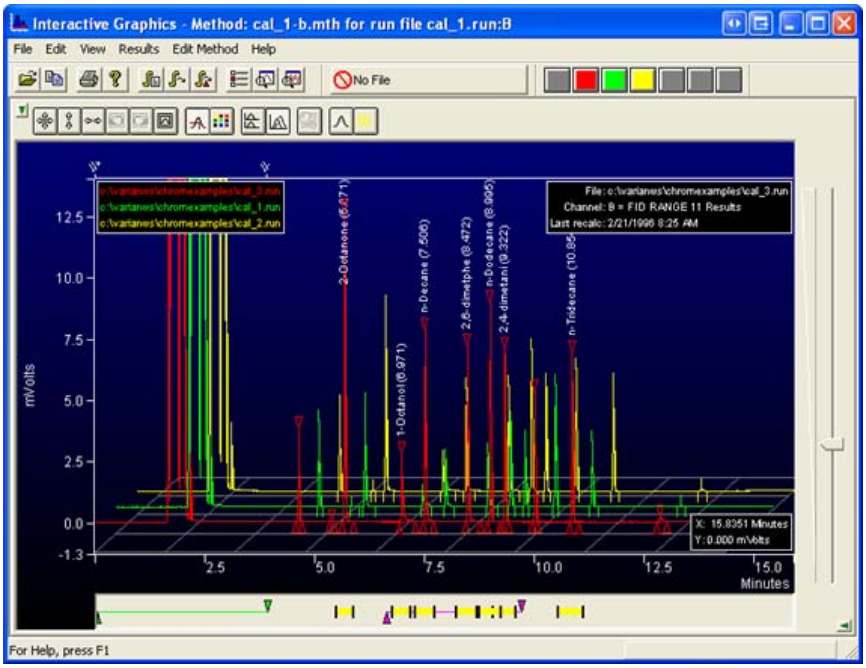
The Locator Window shows the active chromatogram in full scale. Click and drag to view a portion of the chromatogram. The Chromatogram Display Window is updated and the Locator Window shows the zoomed area as a highlighted rectangle. Double-click in this window to return the display to full scale.

Size and position the Locator Window anywhere on the screen. Close the Locator Window by clicking on the button in the upper right corner, by toggling the Locator Display button in the main toolbar, or by deselecting the Locator menu item in the View menu. The display state and position of the Locator Window is displayed the next time Interactive Graphics is opened.

The Chromatogram Display Window

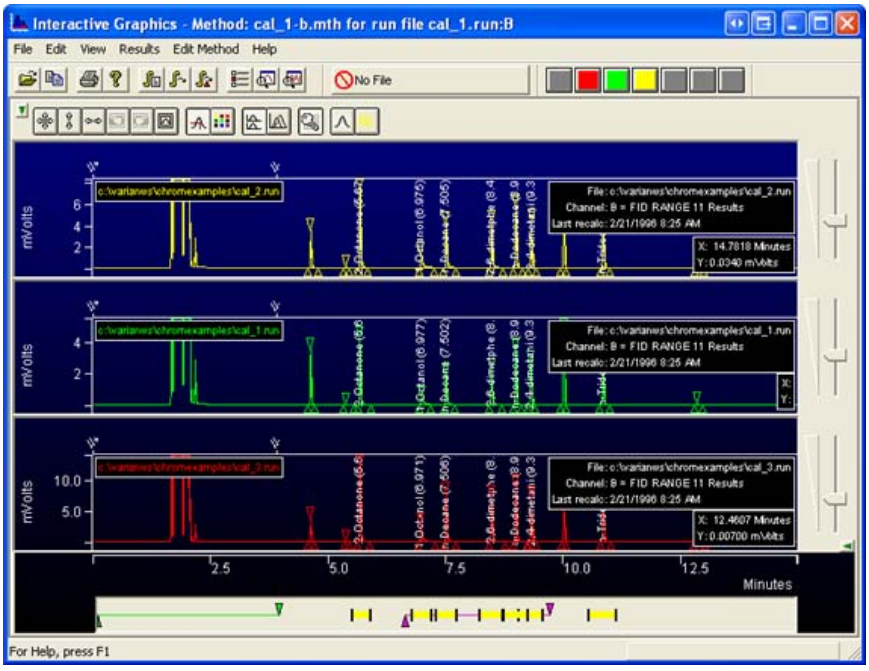
The Chromatogram Display Window shows the portion of the chromatograms that were opened. Click and drag to zoom on a specific area, or click and hold the mouse button to continuously zoom. Hold the control key down while clicking the mouse button to reverse the zooming direction. If the Locator Window is displayed, it is updated to show the zoom area on the full scale chromatogram trace. Double-click in the Chromatogram Display Window to restore the display to full scale.

If multiple chromatograms are open, display them in overlaid or tiled modes. When overlaid, all chromatograms are show on the same time and amplitude axes. By default, the chromatogram traces are offset both in time and amplitude. The offset amounts can be adjusted; see “Changing Viewing Options”.



The black panels contain information about the active or front-most chromatogram. Move the panels with the mouse, and select information by right-clicking in the panel. Move the mouse over an event marker to display information about peak events.

When tiled, each chromatogram trace is displayed separately. All panels have the same time axis, but the amplitude axis of each trace can be independently scaled.



A separate attenuation control appears for each chromatogram.

Right-click on a chromatogram trace, in either mode, to open a menu with options for that chromatogram. Included in these options are report generation and viewing, the option to remove the chromatogram, or bring the chromatogram to the active, or top-most position (in overlay mode only).

Chromatogram Toolbar

Use the toolbar at the top of the Chromatogram Display Window to adjust the chromatogram display settings. See “Chromatogram Toolbar” section for more information.

Attenuation Control

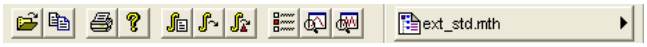
On the right side of the chromatogram display is an attenuation control, similar to a scrollbar. Use it to adjust the scale of the amplitude of the chromatogram. Move the thumb tab up to magnify the vertical scale.

Visual Method Editing Window

The area under the Chromatogram Display Window is the Visual Method Editing Window. Timed integration events and peak table entries are graphically displayed. right-clicking in the panel and select a new event from the menu. After events are inserted, they can be moved and their duration can be edited by moving their endpoints.

Main Toolbar

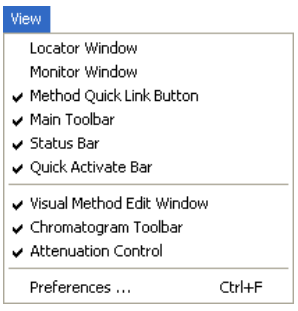
The top of the Interactive Graphics window has the main toolbar. This toolbar provides shortcuts to frequently used functions that are also available as menu items. The main toolbar and the Method Quick Link button can be repositioned in the window or “undocked” and displayed as a floating window by clicking in an empty area in the toolbar and dragging with the mouse.



See “Main Toolbar” and “Method Quick Link Toolbar “for more information.

Changing Viewing Options

Click the View menu to display the options.

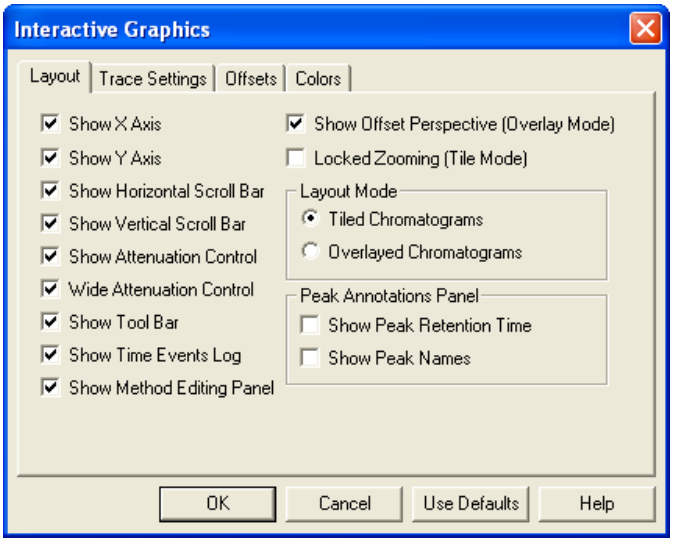


Preferences Dialog Box

Select Preferences from the View menu to display the Preferences dialog box. As changes are made in the Preferences dialog box, the Interactive Graphics display is immediately updated so the change can be previewed.

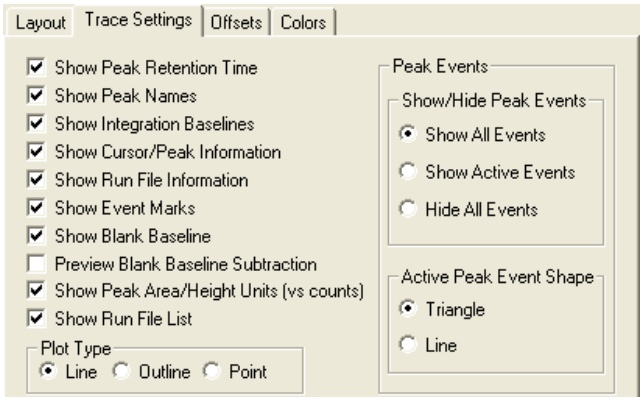
Layout

Layout determines the appearance and behavior of all elements in the Chromatogram Display Window other than the chromatogram trace itself.



Trace Settings

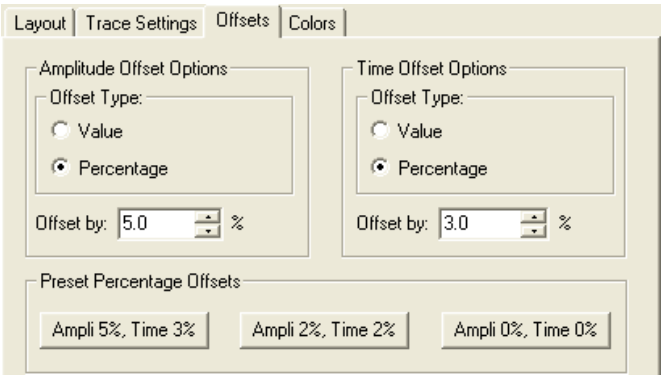
Trace Settings determines the appearance of the chromatogram trace in the Chromatogram Display Window.



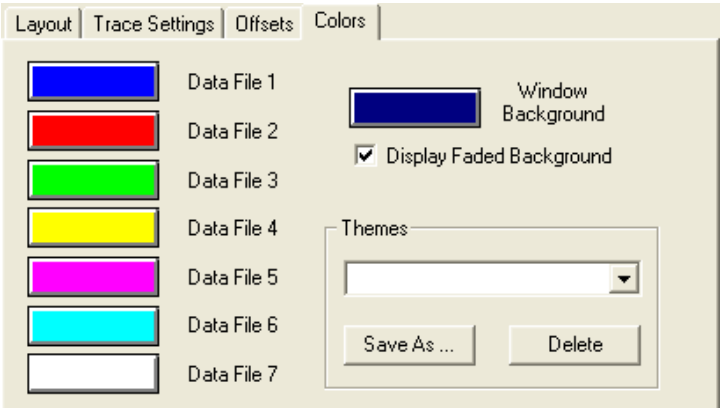
When Preview Blank Baseline Subtraction is selected, the blank baseline stored in the Method can be edited by clicking and dragging points. The chromatogram is drawn as if the baseline has been subtracted. To actually subtract the baseline, you must select Subtract Blank Baseline in the Integration Parameters window in the Data Handling Method Section. If you subtract a blank baseline that was manually edited, is documented in the report.

Offsets

Time and amplitude offsets affect the “3D” appearance of multiple chromatograms when displayed in overlay mode. When offsets are performed by percentage, the distance between traces appears fixed regardless of the scaling. When offsets are determined by a value, the distance between traces changes as the scaling changes.



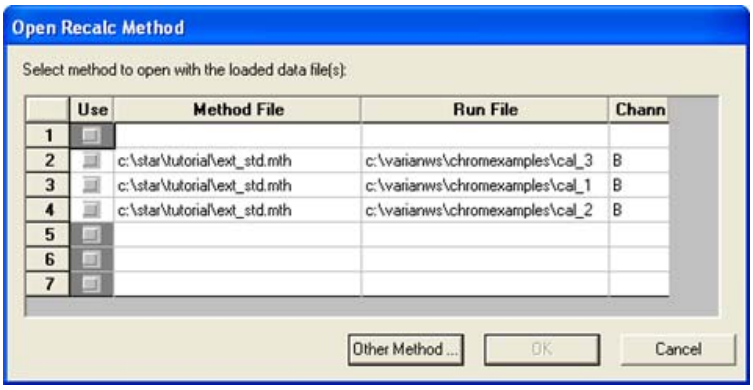
Specify the colors for each of the seven possible chromatogram traces that can be displayed simultaneously. Specify the background color of the Chromatogram Display Window, and if the background is a solid color or is a faded gradient. Save your color settings as a theme, which can be restored.



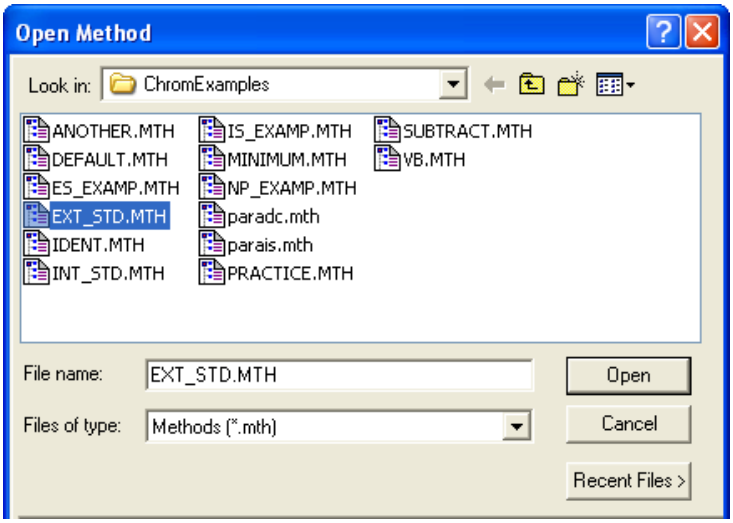
Selecting a Method

When a chromatogram is opened in Interactive Graphics, the Method used to perform the most recent calculation is automatically opened. If this method cannot be found, a new untitled Method is opened.

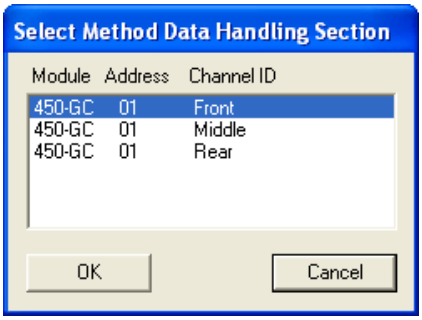
If multiple chromatograms are opened at once and more than one Method was used on the set, you are prompted to select a Method, or browse for another.



To use Data Handling parameters from a Method file stored on disk but not automatically opened, choose it from the File menu. Select the Open Method command. Select the Method containing the desired Data Handling section or select from recently opened methods.



If the selected Method contains more than one Data Handling section, you are prompted to select a section.



To open the Method, originally used with chromatogram(s) currently open in Interactive Graphics, select Open Original Method from the File menu.

Building a Method from the Data File

When a calculation is performed on a Data File using parameters in the Data Handling section of a Method, that Method section is copied into the Data File. Build a new Method from the Data Handling parameters stored in a Data File. Modifications to the new Method do not affect the Method file used when the Data File was acquired. Use the Method created from one chromatogram channel to recalculate results for another Data File.

Select Build Method from Datafile from the File menu. If multiple chromatograms are open, use the cascading menu to select the Data File.

When you select Build Method from Data File, you are prompted for the name of the Method file to be created. This new Method then becomes the active Method.

Changing Data Handling Parameters

The Edit Method menu provides access to the Data Handling Method section. Select the Data Handling section to edit.

Click Method Notes to edit the Notes associated with the Method. Method notes are printed with the method and can be viewed when selecting the method.

Integration Parameters

Integration parameters affect peak detection, peak size calculation and results calculation.

Peak Table

Use the Peak Table to identify peaks. Right-click a column header for formatting options. See the “Filling the Peak Table” section.

Click the Define Peak Windows button to openthe Peak Identification Window.

Peak windows are defined by an absolute time plus or minus a percentage of the retention time.

Reference peaks are marked in the Peak Table with a check in the Ref column. They are used with relative retention time peaks (RRT) to compute relative retention times.

Time Events

Time events affect peak detection and baseline placement. See the “Interactive Editing of Timed Events” section for details on graphically editing time events.

Calibration Setup

Calibration Setup parameters determine the type of calibration and calibration acceptance criteria.

Parameters in this window only apply when a calibrated calculation type is selected. The number of levels determines the number of amount columns displayed in the Peak Table.

In Calibration Setup, specify the action to take when a calibration point is not within the given tolerance, specify the action to take when analysis run is outside the calibrated range, and edit calibration coefficients. Locked coefficients are not updated by calibration runs.

Verification Setup

Verification Setup options affect the behavior of verification runs.

Filling the Peak Table

The fastest way to build a Peak Table is to create one from the detected peaks in the active chromatogram. Select Fill Peak Table from the Edit Method menu.

The Fill Peak Table window is displayed at the top of the screen, above the Chromatogram Display Window.

The Fill table selection automatically adds detected peaks in any selected region in the Chromatogram Display Window to the peak table.

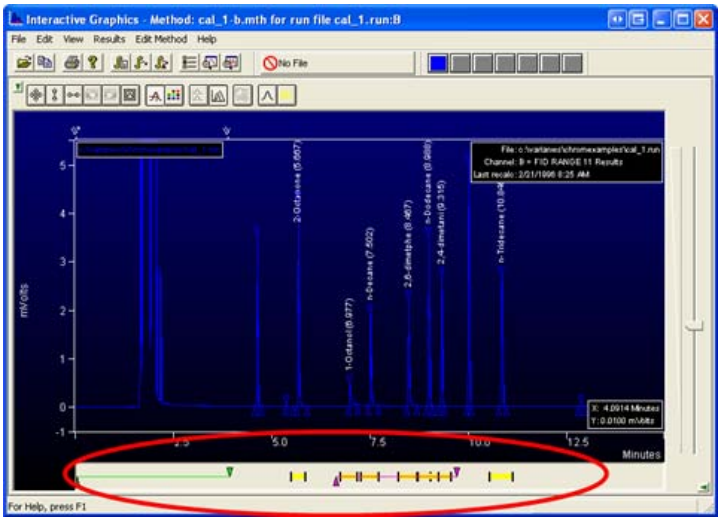
The Fill Peak Table window is nearly identical to the Peak Table window, except that you may click on any peak displayed in the Chromatogram Display Window to add an entry into the table. A default name and peak parameters are entered with the retention time of the selected peak. Click the peaks of interest in the display, zooming and scrolling if necessary to bring the peaks into view. After adding all peaks, click the Save button.

Interactive Editing of Timed Events

Some integration parameters can be set to affect only portions of the chromatogram. This is useful for changes in the chromatographic signal during the course of the run, or to better integrate partially fused peaks, or peaks on a drifting baseline.

Edit these timed integration events from the Time Events window displayed from the Edit Method menu, or graphically place them on the chromatogram display. Peak table entries can also be graphically placed on the chromatogram the same way. Time events added to the chromatogram take effect when a re-integration is performed.

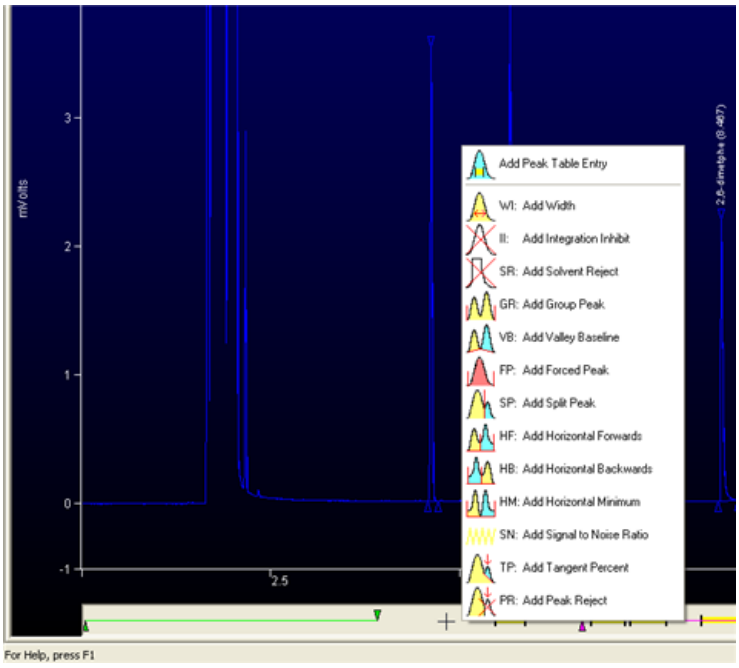
The Visual Method Editing Window is displayed below the chromatogram.



Events that have already taken effect (by reintegrating the chromatogram) are displayed above the chromatogram trace. Double-click a marker to see the entire event table. Event names and values are displayed when the mouse is moved over the event marker.

Peak table entries are displayed as yellow boxes. Double-click a marker to display the peak table.

To add a new time event, right-click in the Interactive Time Events window at the time you want the event to occur.



The event is added to that point. Drag a time range endpoint to change the range. Drag the center of a time range to move the entire range.

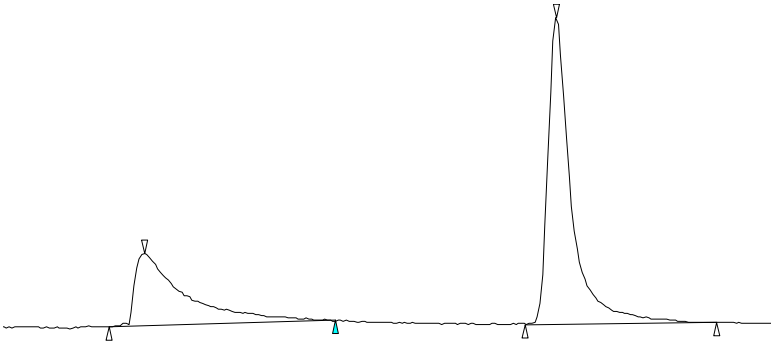
When you change the width of a peak table entry (the yellow boxes), all peak table entries are adjusted. See the “Peak Table” section for more information.

Select multiple events by holding the Ctrl key down while clicking them, or by dragging over the events.

Use the delete key to delete selected events, or right-click on an event to open a menu.

Moving Peak Start and End Points

Peak start and end points are indicated as lines or triangles (depending on the options selected in the Preferences dialog box). Change the position of the points by dragging them.



Right-click a point to return it to its original position or view the peak event information. Manually positioned points are drawn as solid triangles.

When you perform reintegration on a chromatogram with manually positioned peak events, you are asked if you wish to include the changes when calculating results. Click Yes to use the manually placed peak events and reintegrate. Click No to discard the manually placed peak events and reintegrate. Click Cancel to abort reintegration.

If you use the manually positioned peak events, peaks whose areas are affected by the event will be flagged with a “U” (user-modified) in the results report.

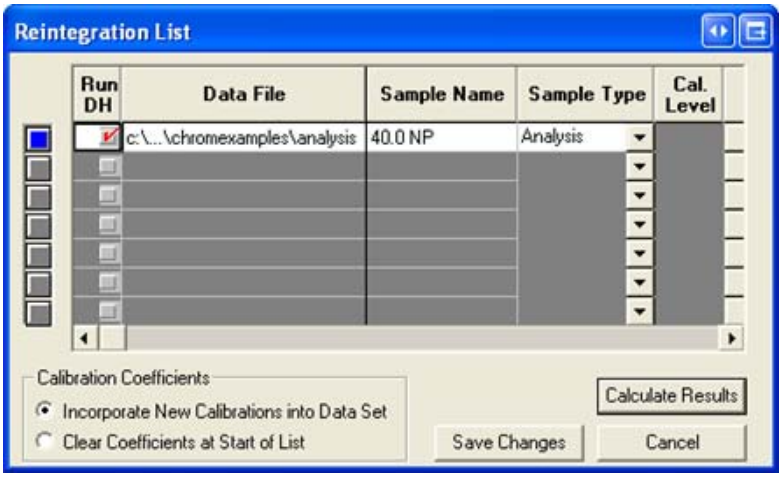
Calculating Results

Results can be calculated for all opened chromatogram channels using the Data Handling parameters in the active Method. Open the Reintegration list by clicking on the button in the Main toolbar, or by selecting it from the Results menu.

In the Reintegration List, select the Sample Type (analysis, calibration, verification, baseline). If results are calculated using an Internal Standard, edit the amount for standard peaks.

You can indicate channels for Data Handling. An unchecked row indicates that no new results will be calculated for the corresponding chromatogram.

If a calibration run is specified, add calibration points to existing data or replace existing data with new calibration points. When you complete the Reintegration List, click Save Changes, and then click Calculate Results.



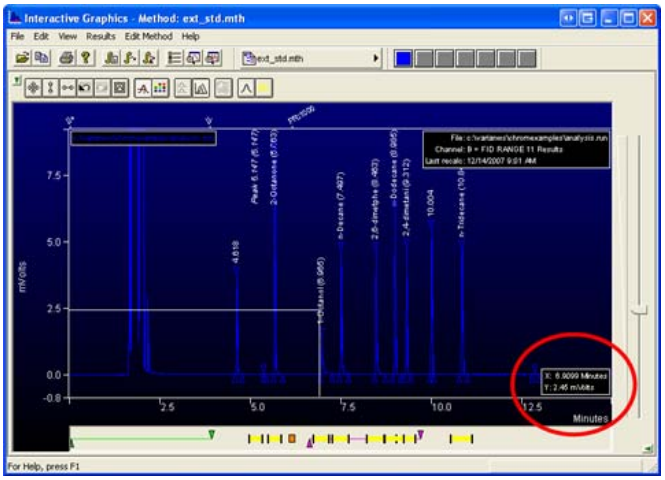
After re-integration, the chromatogram is redrawn with change(s) to peak events. Colored markers indicate timed integration events.

Quickly reintegrate all open chromatograms using the parameters in the Reintegration List by using the Reintegrate Now command, from the Main toolbar or the Results menu.

NOTE: Re=integrate peaks after clearing any manually positioned peak events.

Viewing Results

View results for each peak by enabling the Cursor/Peak Information display from the Chromatogram Display Toolbar. The Cursor/Peak Information display can also be enabled from the Trace Settings tab in the Preferences dialog box.



The Peak Information window is updated with peak data when you move the cursor over the peak.

Right-click the chromatogram to see other results. A menu opens that lists all available report options. This list varies depending on the installed post-run applications. The same list is also available from the Results menu from the Data File name.

Viewing Calibration Curves

If you are performing calibrated calculations (external standard, internal standard or normalized percent), view the associated calibration curves by selecting View Calibaration Curves from the Results menu.

The Calibration Curve window opens if calibration data exists in the active Method. If you have not performed any calibration runs with the active Method, or if you have cleared calibration coefficients without adding any new calibration data, a message box explains that no calibration data exists in the Method.

Printing and Copying the Chromatogram Display

Print the image displayed in Interactive Graphics, or paste it into another document.

To print the image displayed in the Chromatogram Display Window, select Print from the File menu.

To copy the image to the clipboard to use in other Windows applications, click Copy from the Edit menu. The image becomes a picture which can be resized without lose of resolution. You can also copy the image in the zoom window as a bitmap. Bitmaps cannot be resized without becoming distorted.

Copy Picture to Disk to create a Windows metafile that can be imported into Windows graphic applications.

Using Module Information Editor

Module Information Editor

Information about the hardware modules of your instrument(s) can be maintained and included in all data files acquired by this instrument. This information can be included in the reports with the Run Log.

Use the module information editor to define and update the information you want or need to save with your data. The information for module XX is kept in MODULEXX.MDF in the Workstation directory, where xx is the module address.

Edit module information in System Control for any on-line module by clicking Edit Module Info from the Edit menu command or the Edit Module Info Toolbar button. If no module window is active, the Toolbar button displays a list of available modules. Select the desired module. The menu command is disabled if no module window is active.

For routine maintenance. automatically keep track of the numbers of injections in any or all of the module information files. See “Designing Documentation Structures” for details.

The information saved for each module is structured in sections. Each section contains entries, which have the form Item = value. In the table below, the first column shows a typical module information file. The second column describes the elements of this file.

Entry	***Description***
Module	*Section name*
S/N = 1234	*Item1 = value1*
Description = 200-MS Mass Spec	*Item2 = value2*
Name = Old Faithful	*Item3 = value3*
Service	*Section name*
Date First Used = June 5, 1998	*Item1 = value1*
Service Contract = A123456	*Item2 = value2*
Support Number = 800 555 1212	*Item3 = value3*
Date Last Serviced =	*Item4 = value4*
Purchasing	*Section name*
PO# = 123456	*Item1 = value1*
SO# = A12345B	*Item2 = value2*

Limitations

There is no protection against duplicated section names or entries. Duplicated section names or entries cause no harm other than confusion if their contents differ.

There is no built-in mechanism for copying part or all of the information to another module address. If you need to change the address of a module, rename or copy the MODULEXX.MDF accordingly.

Creating a Section

1. Using the cursor or the arrow keys, select a section name or the **'...'** at the end of the list. (The new section will be inserted at the selected location).
2. Click **Add** and enter the name of the section to be created. Bracket are not allowed. Press **OK**.
3. The name of the new section appears, and the next blank line is selected.
4. Press **Add** again to create an Entry in this section.

Deleting a Section

1. With the mouse or the arrow keys, select the section to be deleted - ALL ENTRIES ARE DELETED.
2. Click Delete.
3. You are prompted to confirm the deletion. Press OK, if appropriate.
4. You cannot selectively undo the deletion. If you accidentally delete a section, exit the program without saving the changes. You will lose all edits made since the last save.

Renaming a Section

1. Double-click on a section name. (Alternatively, select a section name and press the Edit button).
2. Enter the new name.

Adding an Entry to a Section

1. Using the mouse or the arrow keys, select the line within the section where you want to insert a new entry. To add an entry at the end of a section, select the blank line at the end of the section.
2. Click Add.
3. Type the item and the value for the entry. To define a new entry like 'Date Serviced = January 12, 1998', type 'Date Serviced' in the 'Key' field, then 'January 12, 1998' in the 'Value Field''. To move to the next field, use the Tab key or the mouse.
4. Press OK to accept your selection. The new entry is added to the list. If it is not correct, double-click on it to edit it.

NOTE: Entries, for which the Value field is left blank, are not followed by an '=' sign. This allows you to enter free-from text, if appropriate. However, you then limit your capability of retrieving information from DATA files retrieve for such lines. Double-click on the blank line at the end of a section to add an entry.

Deleting an Entry from a Section

1. With the mouse or the arrow keys, select the entry to delete.
2. Click Delete. (this button is disabled if you select an empty line).
3. You are asked to confirm your request. If appropriate, press OK. If you accidentally delete an entry, you cannot selectively undo the deletion, but you can exit the program without saving any edits to revert to the last saved version.

Editing an Entry or Renaming an Item

1. Double-click on the entry to modify. Alternatively, select the desired entry and click Edit.
2. Modify the item and/or the value field(s).
3. Click OK to replace the old entry with the modified entry. You cannot selectively undo this action.

Creating a Default Module Information Template

New x.MDF files can be created based on a template file. If MODULE00.MDF is found in the Workstation directory, the new file is a copy of the template. If the template does not exist, the new file is created based on the built-in defaults.

The template is only used to create new files. To recreate an existing .MDF file based on the template, delete the old file (MODULEXX.MDF, where XX is the module address) and edit the module information.

Designing Documentation Structures

First, decide what instrument information you want to track. For example:

- Name and Serial Numbers of components

- Miscellaneous parameters (Column information, and other parameters)

- Usage Information (Injections, and other information)

- Purchase and Warranty Info

- Service History

Decide what information should be attached to which module:

In a system where you only acquire data with an ADCB from instruments, not controlled by the Workstation, attach all information about all system components to the ADCB module.

In a system composed of a 450-GC, an 8200 AutoSampler, and a 220-MS, each module would have a information file documenting its serial number, name, etc. You would likely attach the Column information to the GC module.

Within each Module Information File, create sections named after the major components or operating concepts. You can have as many sections as you want, although there is a 64K limit to the total size of the information saved in a file. Within each section, you can use the Injections field to keep track of consumables. The value of this item is expected to be numerical, and each occurrence of this item will have its value incremented every time the corresponding module starts. As a result, you can keep track of the number of injections performed on a items such as, a column, or a septum.

Septum
Injections = 25
Last Replaced = June 12, 1998
Free-Form Text line ...
Column
Manufacturer = XYZ
Serial Number = A12345
Type = CP-5MS
Length = 30 m
I.D. = .25 mm
Film = 0.25 um
Injections = 123

When you replace a hardware component, zero out (or adequately edit) the associated number of injections.

You can also save free-form text by creating entries with empty Value fields. However, you cannot use the programming interface to retrieve information from such free-form lines.

NOTE: Keep this information current, as the copy of the module information stored in the data files cannot be erased or edited. You may include updates of this information in your Standard Operating Procedures.

Retrieving Information from Data Files

The module information is included in reports if the ‘Run Log’ option is selected.

For Application Programmers only!

Additionally, a function call is available for application programmers to write programs that retrieve module information from run files. This function resides in the WSMDIN32.DLL dynamic-link library, and its "C" prototype and calling syntax are as follows:

```
int PASCAL GetRunInfoString
(
        LPSTR lpRun,        // File Specification for DATA File
        WORD wAddress,      // Module Address
        LPSTR lpSection,    // Section name
        LPSTR lpItem,       // Item name
        LPSTR lpValue       // Buffer for returned entry value
)
```

If the function is successful, it will return the length of the returned entry value.

If the function fails, it will return one of the following error codes:

-3 No info for this Module Address in the DATA file

-2 No such section

-1 No such item

Commands

Buttons

Button	Description
Add	When a section name is highlighted, this opens the Create New Section dialog box. When an item is highlighted, this opens the Create New Entry dialog box.
Edit	When a section name is highlighted, this opens the Rename Section dialog box. When an item is highlighted, this opens the Modify Entry dialog box.
Delete	The highlighted line will be deleted. The user is prompted to confirm this deletion before it is done.

File Menu

The File menu contains the following commands:

Item	Description
Save	Save the contents of the list box into the module information file.
Print	Prints the contents of the list box.
Exit	Aborts the current session. If you have made changes, you will be prompted to save the file before exiting.

Help Menu

The Help Menu provides access to on-line Help and basic Program Information:

Item	Description
Contents	Display on-line Help
About ModEdit	Display basic program information

Dialog Boxes

The Entry Dialog

Use the Dialog box to create and modify entries. Display it by selecting an entry or a blank line and pressing the Add or Edit buttons.

When creating an entry, the item and value fields are empty, and the focus is on the item field. Type in the new item, then use the Tab key or the mouse to switch the focus to the value field.

When editing an existing entry, the item and value fields are filled with their current values. The focus is on the value field, as it is most likely the one you want to modify. If you need to rename the item, use the Shift+Tab key combination or the mouse to move to the item field.

Press OK if you wish to save the new or modified entry, otherwise Cancel.

The Section Dialog

Use this dialog box to create and modify sections. Display it by selecting a section and clicking Add or Edit.

When creating a section, the name field is empty. Enter name of the section.

When renaming an existing section, the name field is initialized with its current value. Type in the new name for the section.

Press OK to save the new or modified entry, otherwise Cancel.

Select

Click a line to highlight it so. Double-click a line to access the appropriate edit dialog directly.

From the keyboard, use the up and down arrow keys to move the selected line up and down. If the list box does not have the input focus, press the up or down arrow key a few times to restore the input focus to the list box.

Security Administration

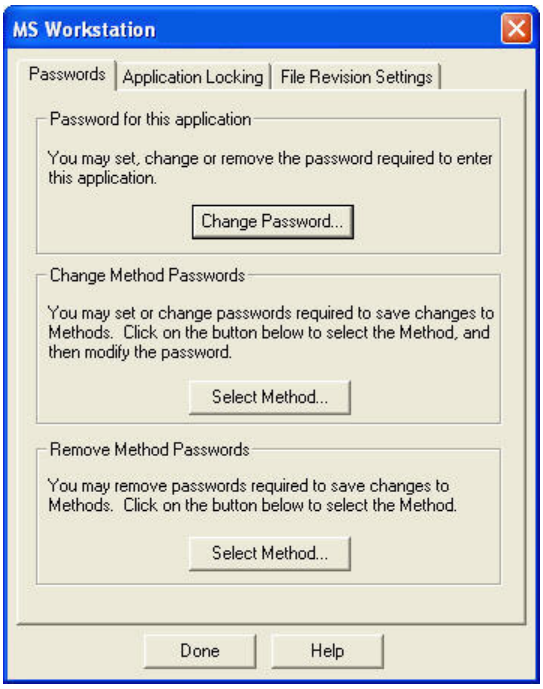
Overview

Security Administration contains three categories of security parameters. These features are tools to comply with 21CFR part 11.

- Passwords
- Application Locking
- File Revision Settings

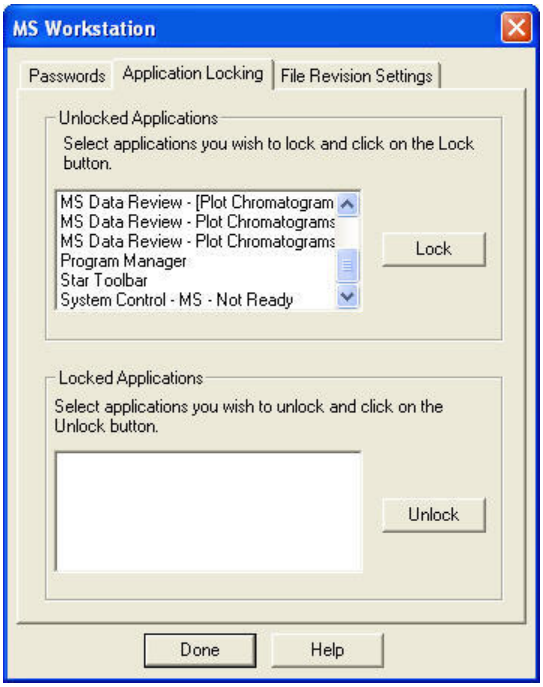
Click the Security button on the Workstation Toolbar to open the Security Administration window.

Passwords



Item	Description
Password for this application	Specify the password required to open Security Administration. NOTE: This password cannot be recovered. so Document it in a secure location.
Change Method Passwords	Method passwords can be added, changed and removed from Security Administration. Click Select Method to browse and select the desired Method. After selecting the method, you are prompted for a new password (if no previous password exists for the Method), or prompted for the old and new password (if the Method already contains a password). NOTE: 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



Item	Description
Unlocked Applications	Lists the top-level windows currently running and not locked. Select the desired ones 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.
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

Item	Description
Require Revision Log entry when changes to Methods are saved.	Prompts you to describe the 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 Data File Revision Log can be included in printed reports.
Enable results deletion from "Open Data File" dialog boxes.	Provides a button in the Open Data File dialog box to allow results to be deleted from a specified channel of a Data File. Results deletion is logged in the Data File's Revision Log. This option only affects standard GC results. GC/MS results will not be deleted.
Disable creation of new passwords in Method files.	When checked, new passwords cannot be added to Methods. Methods already containing passwords will still prompt you for the password before changes are saved.

System Control Toolbar

Main Toolbar

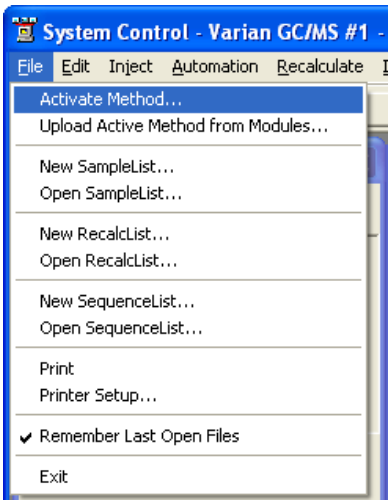
The System Control main toolbar appears at the top of the Configuration and Instrument Windows.

Item	Description
	Creates a new automation file (RecalcList, SampleList or Sequence). You are prompted for the name of the new file.
	Opens an existing automation file. Displays the Open Automation Dialog Box.
	Active Method QuickLink button. Click to display operations that may be performed on the active method, including re-activation (which downloads the method to any modules attached to the instrument).
	Activates a Method. Displays the Active Method Dialog Box.
	Displays the Edit Notes Dialog Box. Notes are displayed in the Open File dialog box and are included in the automation file printout
	Displays the Module Information Editor Dialog Box. Module information is logged in data files generated by the instrument and can be included in reports.
	Displays the Inject Single Sample Dialog Box. Inject a single sample.
	Begins the RecalcList currently open in the instrument. This item is disabled unless a RecalcList has been opened.
	Begins the SampleList currently open in the instrument. This item is disabled unless a SampleList has been opened.
	Begins the Sequence currently open in the instrument. This item is disabled unless a Sequence is open.
	Pause automation. The current run will complete and then automation is suspended.
	Resume automation after a pause. Automation continues at the point that it was suspended.

Item	Description
	Stop automation. Stops the current run, resets all modules simultaneously and suspends the Sequence.
	Instrument status indicator. Shows if the instrument is not ready, running, computing or printing. When the instrument is ready but not running (idle), no status is displayed.

System Control Menu Reference

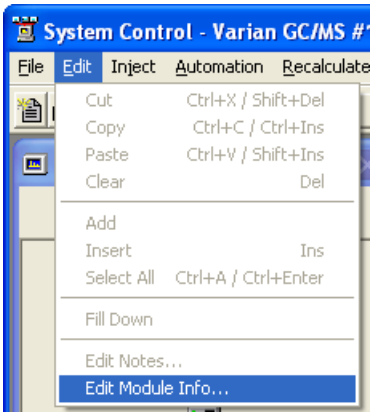
File Menu



Menu Item	Description
Activate Method…	Displays the Activate a System Control Method File dialog box to activate a Method and download the Instrument Control sections to the modules.
Upload Active Method from Modules…	Displays the Save a System Control Method File dialog box to allow you to name the Method that will receive the instrument control sections uploaded from all modules connected to the instrument.
New SampleList…	Displays the Create a New System Control SampleList File dialog box to name a new SampleList.
Open SampleList…	Displays the Open a System Control SampleList File dialog box to open an existing SampleList.
New RecalcList…	Displays the Create a New System Control RecalcList File dialog box to name a new RecalcList.
Open RecalcList…	Displays the Open a System Control RecalcListFile dialog box to open an existing RecalcList.
New SequenceList…	Displays the Create a New System Control Sequence File dialog box to name a new Sequence.
Open SequenceList…	Displays the Open a System Control Sequence File dialog box to open an existing Sequence.
Print	Prints the contents of the active window in System Control.
Printer Setup…	Opens the Workstation Print Setup Dialog Box to select a printer and set options for it. The Varian MS Workstation only uses the

Menu Item	Description
	printer for instrument 1.
Remember Last Open Files	When checked, upon startup,System Control will restore the active Method and any automation files that were open when System Control was last closed.
Exit	Closes System Control. If System Control is in the process of performing a critical operation, you may be prompted before the application is closed.

Edit Menu



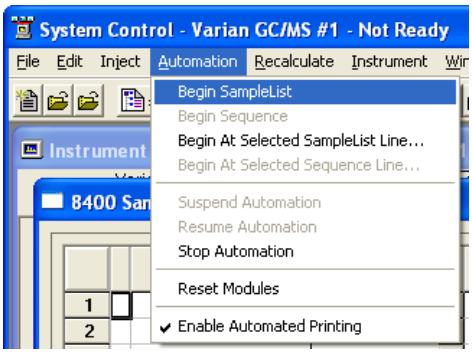
These commands are for use with Sequences, SampleLists, and RecalcLists.

Menu Item	Description
Cut	Deletes a selection and copies it to the Clipboard. Used to remove or move a selected part of a spreadsheet.
Copy	Copies a selection to the Clipboard. Used to duplicate a selection and place the duplicate in a new place (using Paste).
Paste	Inserts previously cut or copied information that was stored in the Clipboard into a spreadsheet.
Clear	Deletes a selection but leaves the Clipboard unchanged.
Add	Adds a new line in a Sequence, SampleList or RecalcList.
Insert	Inserts a new line in a Sequence, SampleList or RecalcList.
Select All	Selects all lines in a Sequence, SampleList or RecalcList.
Fill Down	Copies the the contents of the top cell in a series of highlighted cells to the cells below it. Edit all the cells in a column quickly.
Edit Notes...	Opens the Edit Notes Dialog Box for editing of the notes associated with the Sequence, SampleList, RecalcList, or Method file displayed in the active window.
Edit Module Info...	Opens the Module Information Editor Dialog Box for editing of the Module Information associated with the module displayed in the active window.

Inject Menu

Menu Item	Description
Inject Single Sample...	Opens the appropriate Inject Single Sample Dialog. Inject a single sample without building a Sequence and SampleList manually.

Automation Menu



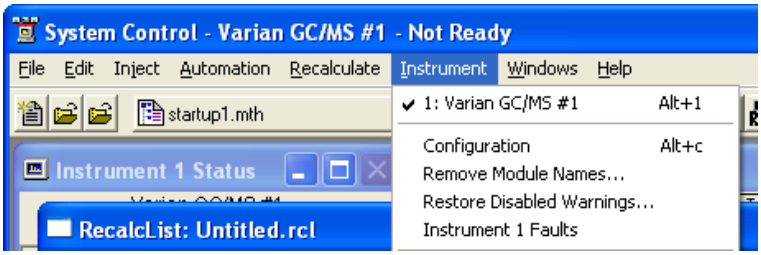
Menu Item	Description
Begin SampleList	Begins execution of the currently open SampleList.
Begin Sequence	Begins execution of the currently open Sequence.
Begin at Selected SampleList Line...	Begins the open SampleList at the selected SampleList line. This item is enabled when a SampleList is open. Upon selecting this menu item, a prompt for the line in the SampleList appears. This is useful when recovering from a power failure that interrupted automation in progress.
Begin at Selected Sequence Line...	Begins the open Sequence at the selected Sequence line. This item is enabled when a Sequence is open. Upon selecting this menu item, a prompt for the line in the Sequence appears. This is useful when recovering from a power failure that interrupted automation in progress.
Suspend Automation	Suspends execution of automation after the current run has been completed.
Resume Automation	Resumes execution of automation after it has been suspended.
Stop Automation	Stops the current run, resets all modules simultaneously and suspends automation.
Reset Modules	Stops the current run, resets all modules simultaneously. Automation proceeds to the next injection after all the modules go to the Ready state.

Menu Item	Description
Enable Automated Printing (checked or unchecked)	Turns on or off the printing of reports automatically generated during any automation action. This is useful when you wish to disable printing (if the printer is out of paper, for example) without having to modify the Print Options portion of the Report Method.

Recalculate Menu

Menu Item	Description
Begin RecalcList...	Begins recalculation of the open RecalcList using the active Method.
Begin at Selected RecalcList Line...	Begins the open RecalcList at the selected RecalcList line. This item is enabled when a RecalcList is open. Upon selecting this menu item, a prompt for the line in the RecalcList appears. This is useful when recovering from a power failure that interrupted automation in progress.
View Calibration Curves...	Opens the Open a Method File to View Curves dialog box to view calibration curves that are stored in a Method file.

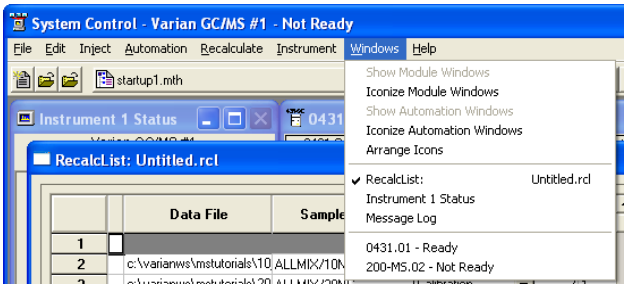
Instrument Menu



The Instrument Menu commands switch the display between the configuration screen and the instrument.

Menu Item	Description
#:instrument name	Displays the Instrument Status window and Status and Control windows for the named Instrument. i.e. Varian GC/MS #1
Configuration	Displays the Configuration window.
Instrument # Faults	Displays the Instrument Faults dialog box, showing recent and self-test messages and faults. The list of faults may be printed from this dialog box.
Setup Ethernet Communications	Available if an optional module driver is installed that uses Ethernet to communicate with the device. See the Operation Manual for your module driver for a detailed description if applicable. Allows set-up of the communication between the 450-GC and Mass Spectrometer
Setup COM Ports	Available if an optional module driver is installed that uses Serial I/O to communicate with the device. See the Operation Manual for your module driver for a detailed description if applicable.
Setup ADC Board Ports	Opens the Setup ADC Board I/O Ports Dialog Box to configure the ADC Board base address and determine the Switch S1 settings for each ADC Board. Applicable only if the ADC Board module driver is installed.

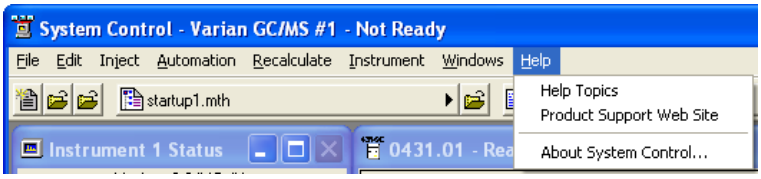
Windows Menu



Menu Item	Description
Show Module Windows	Opens the Status and Control windows for all modules. It is disabled when all the windows are open, even if some are hidden under others.
Iconize Module Windows	Iconizes the Status and Control windows for all the modules in the Instrument. It is disabled when all the windows are iconized.
Show Automation Windows	Opens the windows for all open automation files. It is disabled when all the automation windows are open, even if some are hidden under others.
Iconize Automation Windows	Iconizes the windows for all the automation files in the Instrument. It is disabled when all the windows are iconized.
Arrange Icons	Arranges the icons, if any, in a row at the bottom of the System Control window.
Sequence:	Opens the window for the selected file or moves it

Menu Item	Description
SampleList: RecalcList:	to the front. Used to display the open Sequence, SampleList, or RecalcList.
Instrument Status Message Log Configuration Log (only if Configuration window is open)	Displays the corresponding window for the instrument or moves it to the front. Used to see the instrument status, Message Log, or Configuration Log.
Module Window (name varies depending on module)	Displays the Status and Control window for the chosen module or brings it to the front.

Help Menu

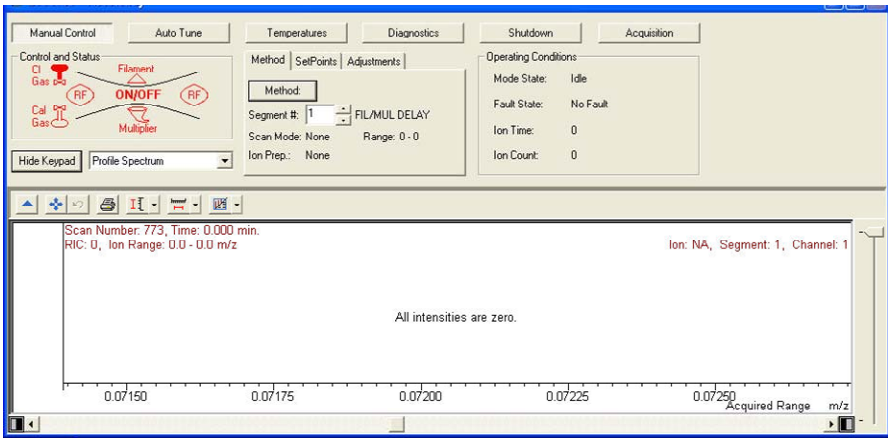


Menu Item	Description
Help Topics	Displays the help for what you are viewing.
Product Support Web Site	If you have Internet access and a web browser on your computer, this option automatically opens the Varian MS Workstation Product Support Web Site. The site has the latest software and documentation updates for the Varian MS Workstation products, and additional notes, tips, and answers to frequently asked questions. Visit this site periodically to see if new information is available that may be pertinent to you.
About System Control	Displays the About Box for the System Control application. The About Box contains information about the software version, installation information, and a list of the instrument control modules that you have installed.

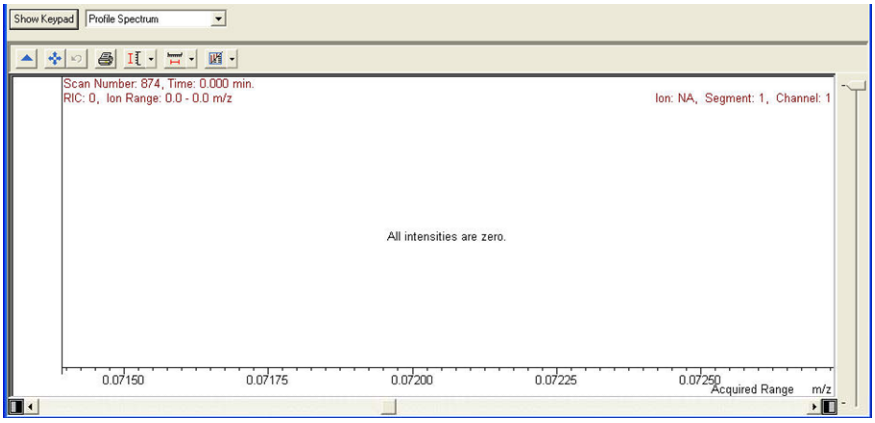
MS Instrument Control Command Reference

200-MS Module Dialogs

200-MS Module Keypad Dialog



Click **Hide Keypad** to expand the chromatogram.



Spectrum Toolbar

 Click the blue arrow to hide the toolbar. Click the upper left of the full screen display to restore the toolbar.

 Click full scale to normalized to chromatogram. Double-clicking the chromatogram does the same.

 Click to return the xy axes to the previous scale.

 Click spectrum plot to open a preview of the spectrum.

 Click scale to choose between Auto Scale and Fixed Scale Intensity.

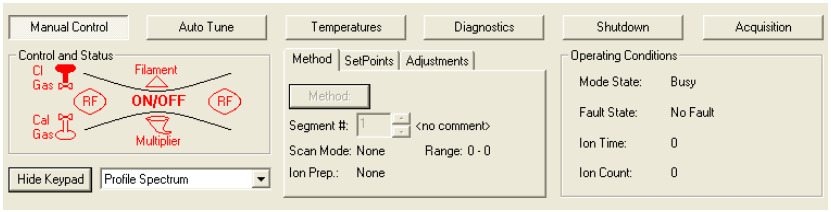
 Click mass range to choose between Acquired Mass Range, Fixed Mass Range, or Maximum.

 Click to switch graphics or text displays of ion intensity and status information.

 Click select preferences to change the color of the chromatogram display, labels, axes, font, and other features.

 Click Report Preferences to choose the chromatogram and spectra options for the standard report.

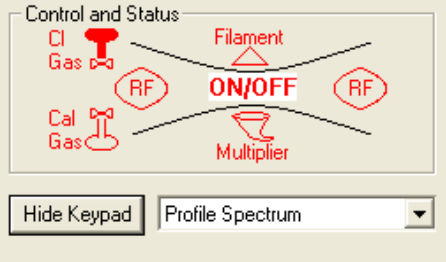
MS Module Window



Item	Description
Manual Control	Click Manual Control to turn the trap controls (rf, Filament, and Multiplier) on or off and to open the CI and Cal gas valves. Also adjust the rf response, the CI gas pressure, and the Cal gas pressure. Use this to select the current trap filament and to adjust the axial modulation voltage. Although scans may be taken and displayed under method conditions of any one of the MS Method segments, data may not be acquired while in this mode. To acquire data, Acquisition Mode must be selected.
Auto Tune	Tune the instrument, including the multiplier setting, mass calibration, and trap function calibration.
Temperatures	Change the temperature of the ion trap or transfer line. Bake out to remove volatile materials absorbed on electrode surface.
Diagnostics	Check the system for status and faults.

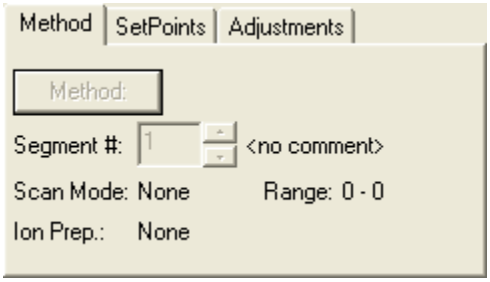
Item	Description
Shutdown	Shutdown for routine maintenance or for an extended period.
Acquisition	Acquire data for a single sample or an automated list .

Manual Control



Item	Description
On/Off	Turn on or off the ion trap (the filament, rf and multiplier).
RF	Turn on or off the rf
Filament	Turn on or off the filament.
Multiplier	Turn on or off the multiplier.
CI Gas	Open the valve to turn on the CI gas.
Cal Gas	Open the valve to turn on the Cal gas.
Hide Keypad	Remove the upper portion of the screen display so that the lower portion is expanded.
Display Selection	Select from to view the spectrum in profile or centroid mode.

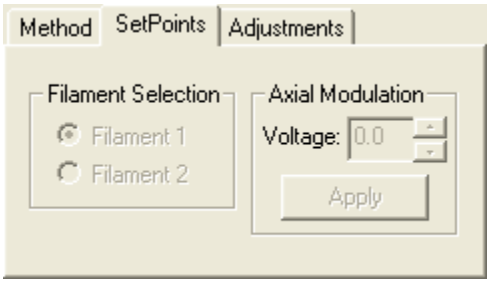
Instrument Settings



Item	Description
Method button	Opens the Method Editor program.
Segment # box	Select the current segment of the active method.
Scan Mode	Ionization mode of the current segment, such as EI-Auto.

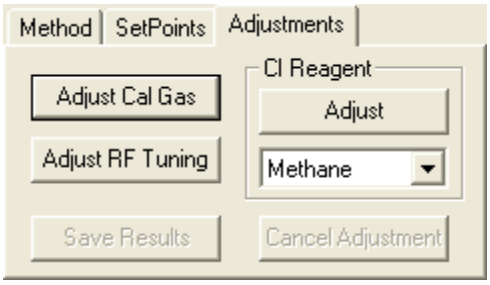
Item	Description
Ion Prep.	Ion preparation method of the current segment, such as MS/MS.

SetPoints Tab



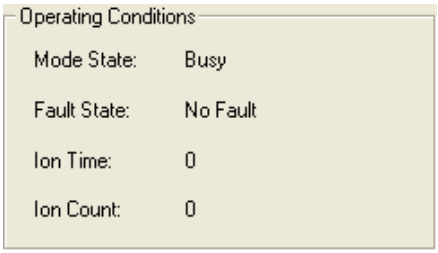
Item	Description
Filament Selection	Click to select the current filament. The MS has 2 filaments so the system can be used if one burns out.
Axial Modulation Voltage	Select the voltage to apply to the upper end caps. *Recalibrate the mass axis when you change this value.*
Apply button	Apply changes you make to the Axial Modulation Voltage. If the voltage edit control has the focus, press enter to apply the changes.

Adjustments Tab



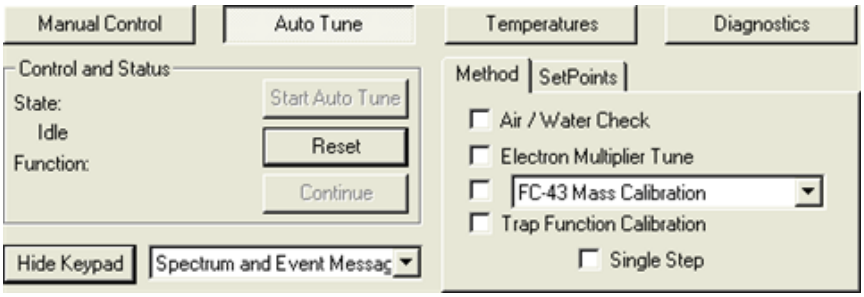
Item	Description
Adjust Cal Gas	Click to adjust the cal gas pressure.
Adjust rf Ramp	Change the rf setting for the instrument by turning the screw at the bottom front panel.
Adjust	Set the proper CI reagent pressure for CI analysis. The pressure is very dependent on the reagent gas used.
Reagent Gas Selection Box	Choose which CI gas you are using.
Done	Used when you complete your adjustment.

Status



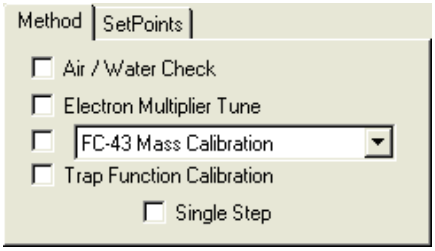
Item	Description
Mode State	Indicates what function the MS is performing, such as scanning or adjusting cal gas.
Fault State	Indicates if a fault has occurred.
Ion Time	Indicates the ionization time of the last scan.
Ion Count	Indicates the ion count of the last scan.

Auto Tune



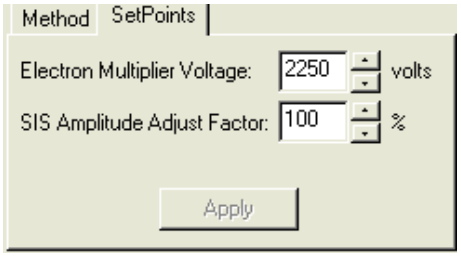
Item	Description
Start Auto Tune	Begins the sequence that tunes the instrument. Only checked boxes are executed.
Reset	Stops the auto tune process.
Continue	Starts the next selected function if the single step option has been checked.
Hide Keypad	Causes upper portion of the screen to be removed so that the lower portion can be expanded in the display.
Display Selection	Select the display.

Method



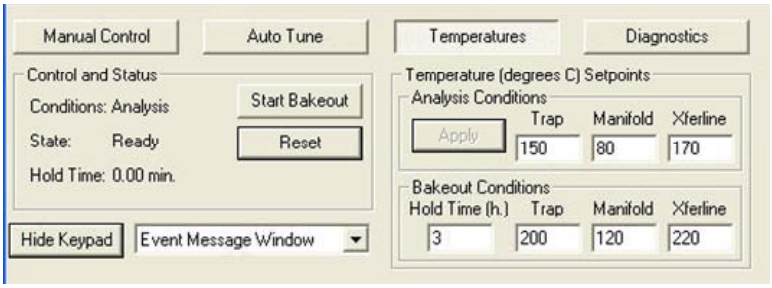
Item	Description
Air/Water Check	Measures the air and water content of the trap, to determine if there is a leak.
Electron Multiplier Tune	Autoset the electron multiplier voltage.
FC-43 Mass Calibration	Calibrate the mass axis. Choose Straight Line or FC-43.
Trap Function Calibration	Calculate the waveforms for CI, MS/MS and SIS.
Single Step	Observe each step in the auto tune process. Use Continue to proceed after each step.

SetPoints



Item	Description
Electron Multiplier Voltage	Manually adjust the Final Gain Setting, which is determine from the Auto Tune check.
SIS Amplitude Adjust Factor	Adjust each trap system for optimum ion sensitivity and ejection. The voltage adjustment range is between 50 to 200%. The default is 100%.

Temperatures

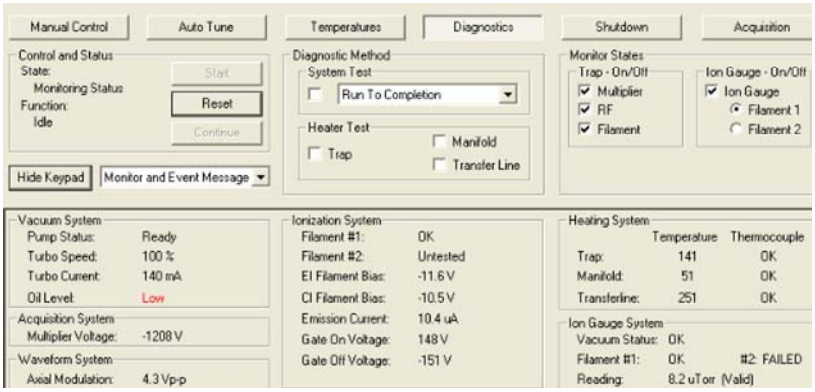


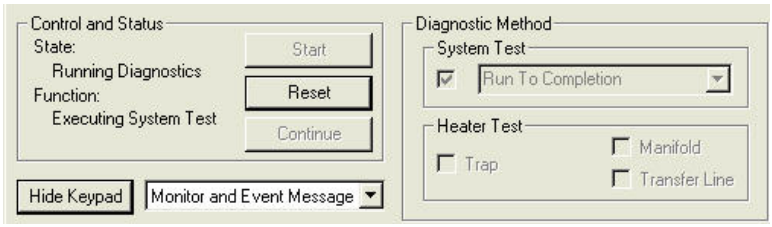
Item	Description
Start Bakeout	Execute the bakeout conditions, which removes volatile material from the ion trap surface.
Reset	End a bakeout before the specified time.
Hide Keypad	Hide the upper portion of the screen and expand the lower.
Analysis Conditions	Set temperature for trap, manifold and transfer line. Click Apply to initiate conditions.

Item	Description
Bake out Conditions	Hold Time specifies the number of hours for bake out. Under Trap, set the bake out temperature, such as 220 °C. The manifold bakeout temperature is fixed. The transfer line bakeout temperature matches the analysis temperature.

Diagnostics Mode

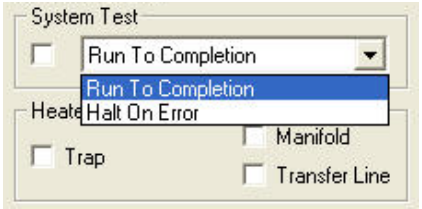
NOTE: Oil Level readback is only on the 225-MS





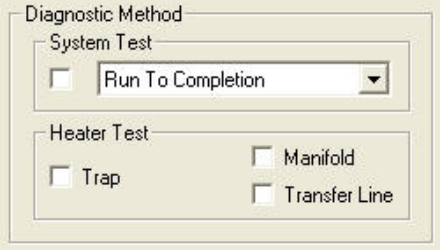
Item	Description
Start	Click Start to execute the desired test
Reset	Cancel a test executed with Start.

Diagnositcs Method (System Test)



Item	Description
Run To Completion	Click to run all tests without stopping.
Halt On Error	Halts the system checks when an error is detected.

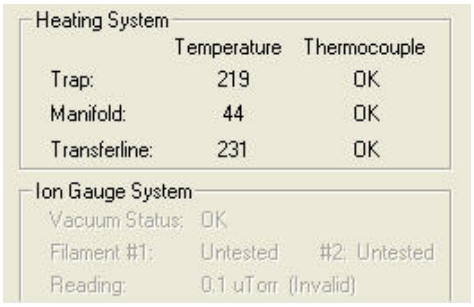
Diagnostics Method (Heater Test)



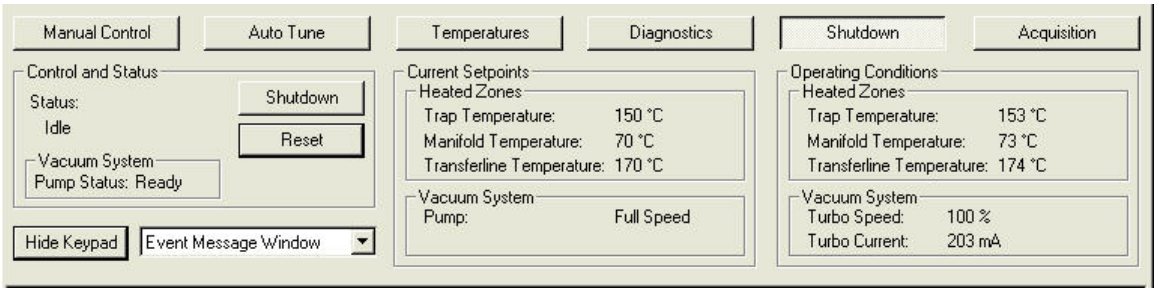
Item	Description
Trap	Tests the Ion Trap heater element May take up to 13.5 hours to complete.
Manifold	Tests the Manifold Heater element.
Transfer Line	Tests the Transfer Line heater element.

Monitor States

Item	Description
Multiplier check box	Display the voltage (center left) on the multiplier when on.
RF check box	For Service Engineers.
Filament check box	Display the status of the system filaments (upper right).
Ion Gauge check box	View the vacuum status using the filament selected by the Filament Radio Button.
Filament	Select a filament and view the ion gauge vacuum system test.

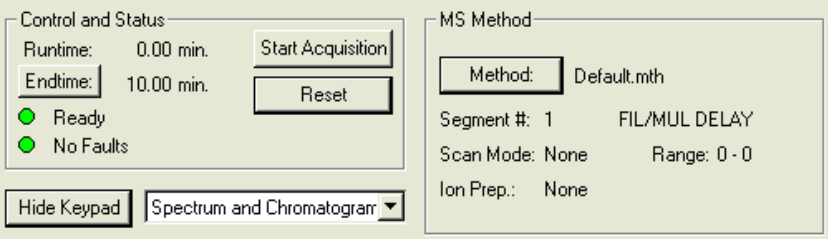


Shutdown Mode



Item	Description
Shutdown button	Orderly shuts the system down. The pump speed is slowly reduced and the heaters are turned off so that the system slowly cools.
Reset button	Brings the system back to a ready state if the Shutdown procedure was started. Restarts the pumps and turns on the heaters.

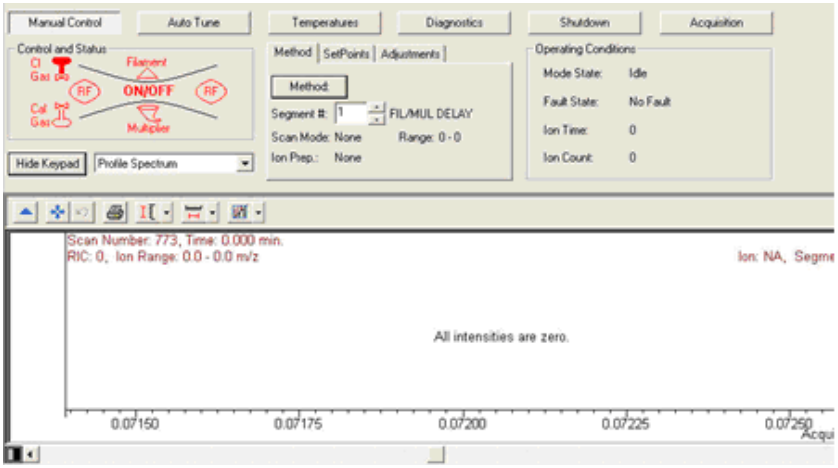
Acquisition Mode



Item	Description
Start Acquisition button	Click to start the analysis.
Reset button	End the acquisition and reset the conditions to their initial conditions.
End time button	Click to increase or decrease the end time of the analysis.
Hide Keypad button	Hide the upper portion of the screen and expands the lower portion.
Display Box Selector	Select chromatogram, spectra, or both.
Method button	Open the Method Editor with the active method. Edit the method and then return to this screen for analysis.

MS Instrument Window

The MS Instrument Window



System Control has four major sections: the System Control Menu bar, System Control Toolbar, Keypad Dialog, Chromatogram and Spectrum Toolbar, and Spectrum Display.

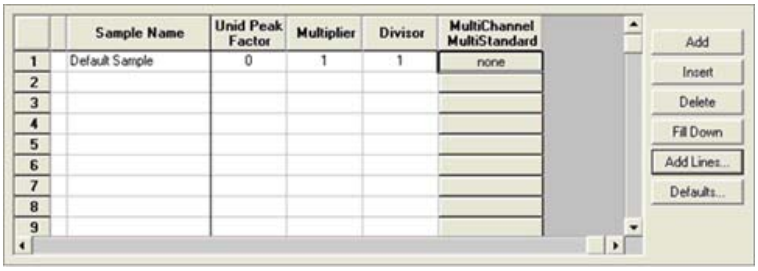
File Menu

Activate Method: Choose a method from those already prepared. This will set the conditions for the GC, MS, AutoSampler and data handling. Other sections will also be activated if they are part of the method.

Upload Active Method from Modules: Save the conditions from the existing modules in a new method. The active method is converted to the conditions of the active modules.

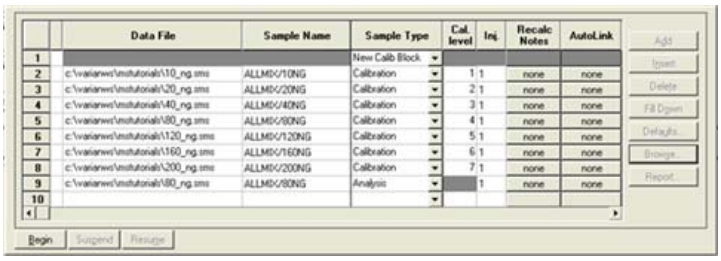
New Sample List: Open the dialog box to create a sample list.

Open Sample List: Select and activate an existing sample list. The sample list dialog box is displayed.



New Recalc List: Open the dialog box to create a recalculation list.

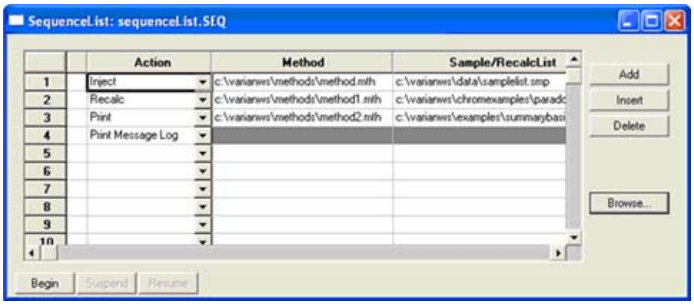
Open Recalc List: Select and activate an existing recalculation list. The Recalc list dialog box is displayed.



NOTE: Process a Recalc List either in System Control or in MS Data Review. In MS Data Review use the menu command **Quantitation… Process/Review Recalc List**. Although, processing a Recalc List takes more time when done from System Control it allows AutoLink functions such as automated reporting with Custom MS Reports templates.

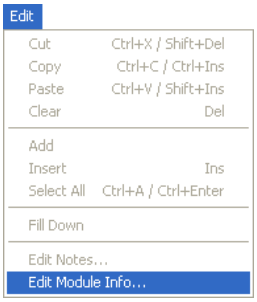
New Sequence List: Open the dialog box to create a sequence list.

Open Sequence List: Select and activate an existing sequence list. The sequence dialog box is displayed.

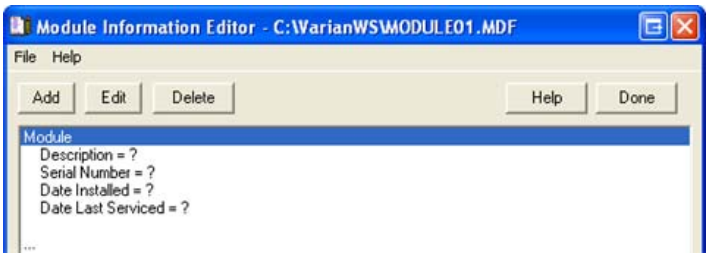


Edit Menu

Click the **Edit** menu and highlight **Edit Module Info.**



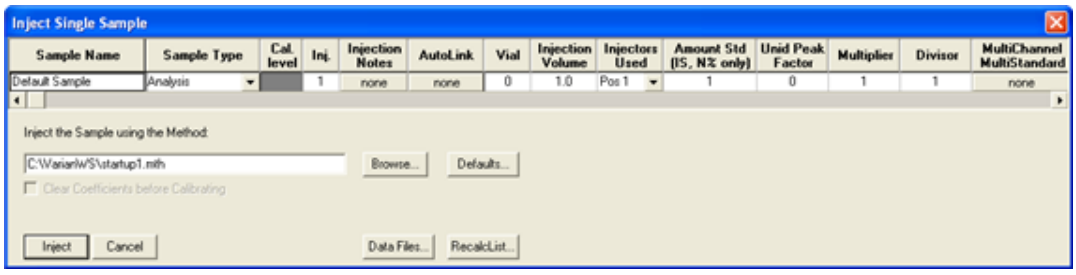
Each module in your system (450-GC, 220-MS, etc.) has a message log and documentation screen. Use the Module Documentation to keep a record of performance, maintenance, hours used, or other comments.



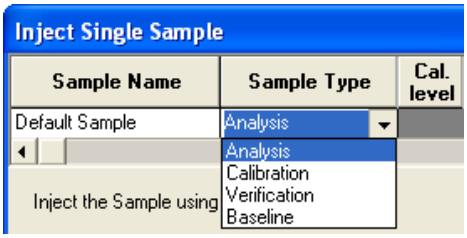
Use the Add, Edit, and Delete buttons to record information about the MS module.

Inject Single Sample Menu

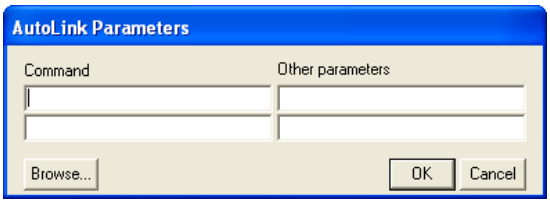
Use this command to provide sample information before an injection. The following is the dialog box. The MS module window must be in acquisition mode for the system Not Ready to convert to Ready. If using an AutoSampler, click **Inject** in the bottom left corner.



Change the sample type by double-clicking the field below Sample Type. The following displays the choices.



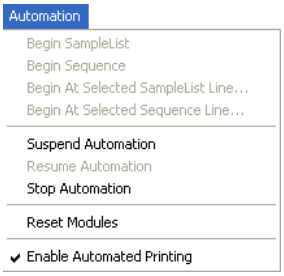
Use the same procedure for Injection Notes. Any notes that you enter here are saved with the data file. The AutoLink button works in the same way.



Commands entered here execute a program after the data file is acquired. For example, this can be a program to activate Custom MS Reports to print the sample reports. To run a Custom MS Report in automation enter the directory path and the name of the Custom MS Report template (for example C:\VarianMS\EPA525.swt). Store Custom MS Reports templates in the VarianWS directory. Use browse command to select the command executable file. Select OK after you made your selection.

Automation Menu

The following is the **Automation** menu.



Begin Sample List: Starts an automation at line 1 and ends at the last line.

Begin Sequence: Change methods and sample list during an automation. An example of this is running a set of samples using EI and then the same set of samples using a different MS method for CI.

Begin At: Starts an automation at a selected line and runs until the last line is completed.

Suspend Automation: dtops an automation at its last completed sample.

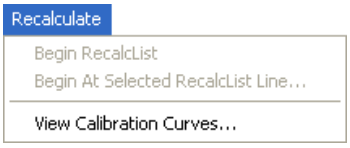
Resume Automation: Starts the automation after it was suspended. It starts where it was suspended.

Stop Automation: Ends the automation action.

Reset Modules: Puts the modules in the ready states.

Enable Automated Printing: Printer functions work during an automation.

Recalculate Menu

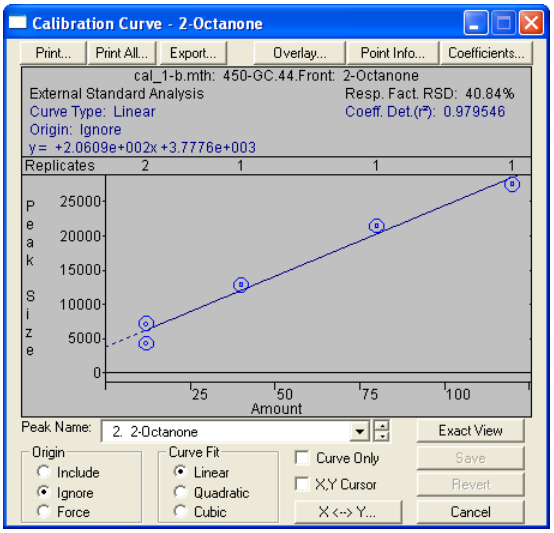


Recalculation may be performed in System Control or in MS Data Review under the menu command Quantitation… Process/Review Recalc List. Also that processing of a Recalc List takes more time when done from System Control than in MS Data Review but allows AutoLink functions, such as automated reporting with Custom MS Reports templates.

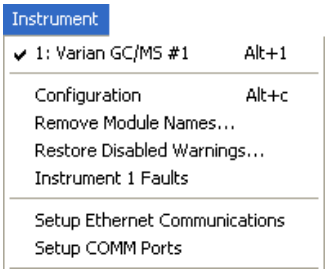
Begin RecalcList: Start an automated recalculation. A recalculation list must be prepared and selected. A New Recalc list may need to be made.

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 any curve for the calibrated compounds in the active method. An example of the calibration curve screen follows. For a complete explanation of this screen, go to the Quantitation section of the *MS Workstation Software Reference Manual*.



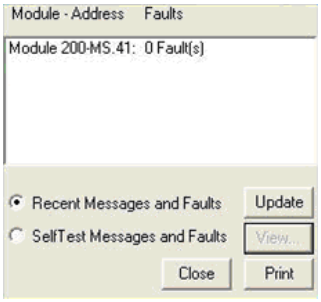
Instrument Menu



Varian GC/MS #1: The name of the configured instrument.

Configuration: Add new modules to the existing instrument..

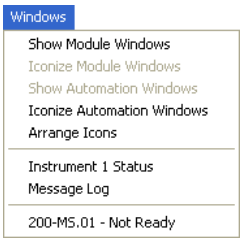
Instrument 1 Faults: Displays any faults in any of the modules contained in Instrument 1. An example of this screen follows. Use the update key to periodically check for new faults without opening and closing the dialog box. MS faults are not reported in this window.



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

Windows Menu

View any window associated with the system control.



Show Module Windows: See all of the windows for all configured modules. In this example the module available is the 200-MS.

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

Show Automation Windows: View any automation screen, which include the Sample list, Recalc list, and Sequence list.

Arrange Icons: Arranges the displayed icons, in a row at the bottom of the System Control window.

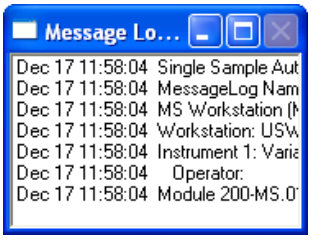
Sequence List: Display the active sequence list.

Sample list: Display the active sample list.

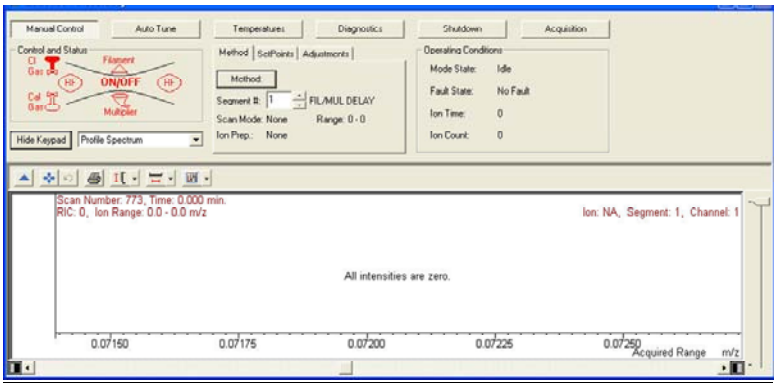
Recalc list: Display the active recalculation list.

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

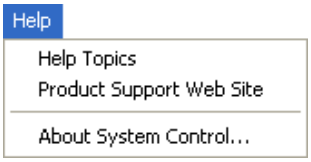
Message Log: View the event log for the MS module. All error messages are displayed.



MS Module: Display the MS module control screen.

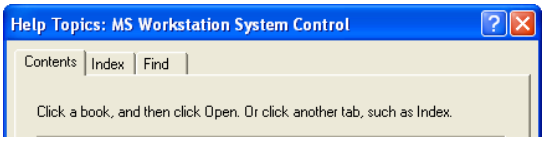


Help Menu

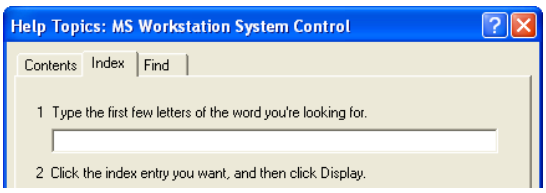


Click Help Topics to show the Help dialog.

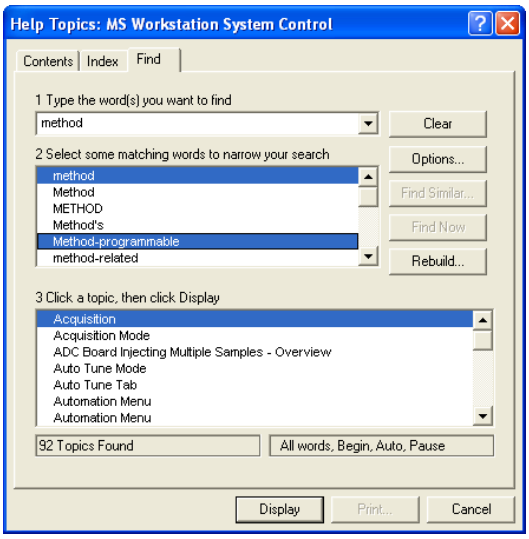
Click a book under the Contents tab to show related topics.



Under the Index tab, type one or more words or the beginning of a word. Then, select an entry and click Display.



Under the Find tab, type a word or select a word that was previously searched. Then select matching words to narrow your search. Finally, select a topic and then click Display.

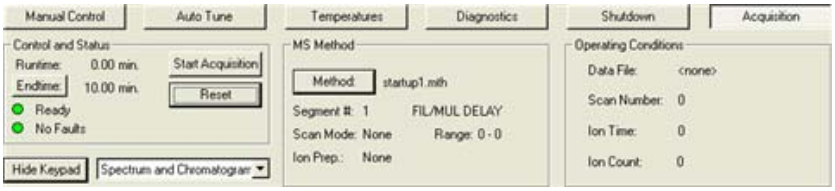


System Control Toolbar

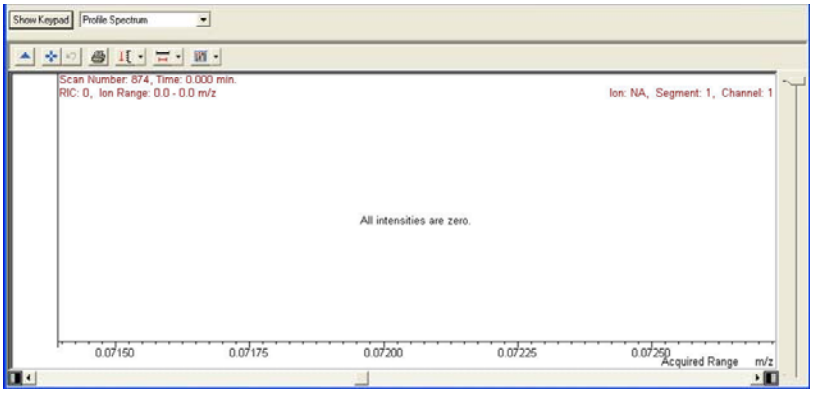
The system control toolbar is near the top of the screen.

	Create a new automation file
	Select a new automation file
startup1.mth	View/edit or print a method
	Activate a method.
	Edit notes for an automation file.
	Edit module information for any module that is online, such as the 200-MS or the 450-GC.
	Inject a single sample.
RCL	Start an active recalculation list.
SMP	Start a created sample list. NOTE: the list must be selected
SEQ	Start a sequence list.
	Suspend a list that is running.
	Begin a list.
	Stop a list that is running.

MS Module Keypad Dialog

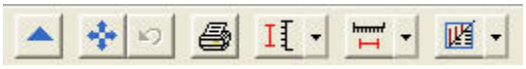


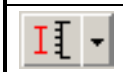
Clicking **Hide Keypad** to only display the spectrum.



Click **Show Keypad** to display 200-MS Module Modes **:** Manual, Auto Tune, Temperatures, Diagnostics, Shutdown, and Acquisition. See 200-MS Module Modes for details.

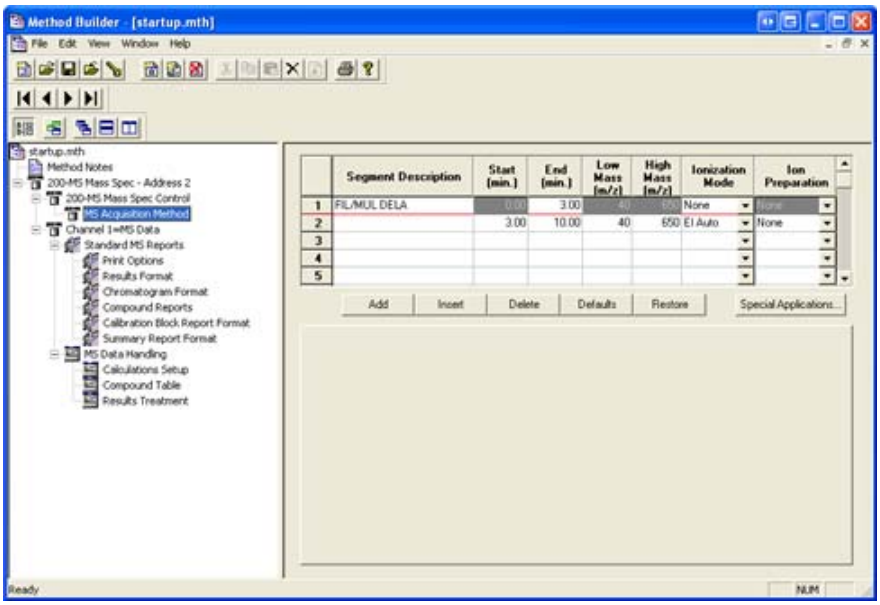
Spectrum Toolbar



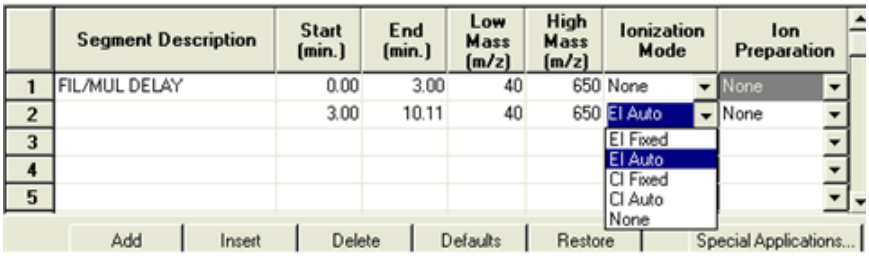
	Hide the toolbar. Click the upper left of the screen to restore the toolbar
	Normalize the chromatogram in the vertical and horizontal directions by clicking the full scale button. Double-click the chromatogram to do the same
	Return the xy axes to the previous scale
	Previewing the spectrum before printing it.
	Select between Auto Scale Intensity and Fixed Scale Intensity.
	Select Acquired Mass Range, Fixed Mass Range, or Maximum.
	Switch between graphics and text displays of ion intensity and status information

MS Method Command Reference

Spreadsheet Editing

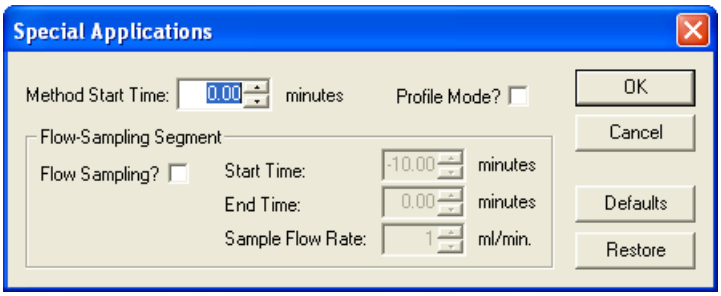


Item	Description
Add	Duplicates MS parameters of the last segment and adds it to the end of the current table.
Insert	Inserts a row before the one currently selected with the parameter values of the highlighted row.
Delete	Deletes the currently selected row.
Default	Inserts system default parameters.
Restore	Inserts parameters present when the method was first opened, or last saved.



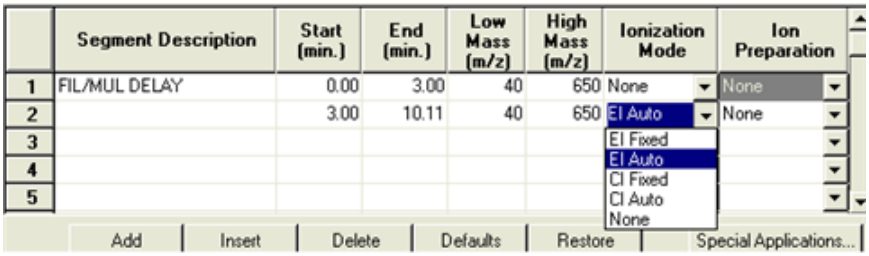
Item	Description
Segment Description	Comment Line. 20 characters can be entered.
Start Time	Start time of segment in minutes. 0.00 to 649.99 min.
End Time	Time segment will be terminated. 0.10 to 650 min.
Low Mass	Lower end of mass range to be acquired. 10 to 650 m/z.
High Mass	Upper end of mass range to be acquired. 10 to 650 m/z.
Ionization Mode	Method of ion formation in trap.
Ion Preparation	Options applied after ionization to alter the ions stored in the trap before analysis.
Special Applications	To specify data acquisition in Profile mode (vs. Centroid) or to specify a pre-acquisition flow sampling period.

The Flow Sampling Segment



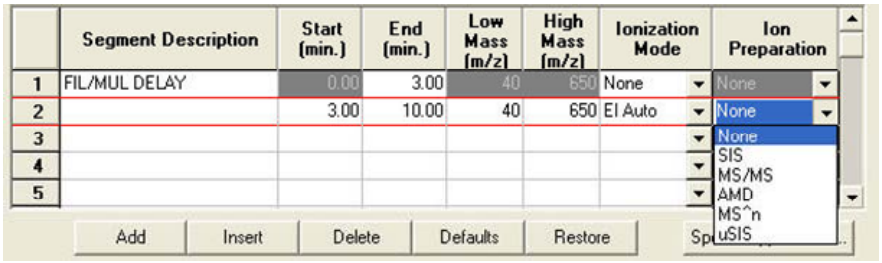
Item	Description
Method Start Time	The time to flush the system before sample collection begins plus the actual sampling time. Time of -30 to 0 minutes may be entered.
Flow-Sampling Start Time/ End Time	The duration of the actual sampling, from -10.00 to 0 minutes. If time = 0, no flow sampling is done.
Sample Flow Rate	Set from 1 to 100 mL/min. Must be equal to value set on EMFC in manual mode. If EMFC is set to auto mode, the sample flow rate specified will be downloaded at the start of the injection

Ionization Mode



Item	Description
EI-Fixed	Ions formed by electrons for a time set in method.
EI-Auto	Ions formed by electrons for time calculated from AGC function
CI-Fixed	Ions formed by collisions with CI reagent ions for time set in method.
CI-Auto	Ions formed by collisions with CI reagent ions for time calculated from previous scan.
None	Selected when hardware is to beturned off (i.e. solvent peak elution)

Ion Preparation



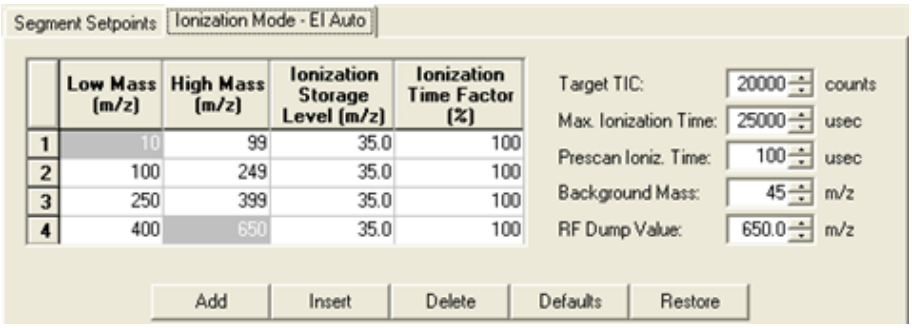
Item	Description
SIS	Selectively trap ions, a range of ions or eject ions.
MS/MS	Isolate and dissociate an ion or ions.
AMD	Find optimum dissociation conditions for MS/MS for single percursor ion.
MS^n	Use two to five percursor ions for sequential dissociation.
uSIS	Unit mass isolation of 1 to 10 ions.

Segment Setpoints

Item	Description
Scan Time	The duration of each scan (in seconds). Values from 0.10 to 5.00 seconds per scan. Below the scan time input box is displayed the number of micro scans per scan for the selected mass range and scan time.
Multiplier Offset	Multiplier offset (relative to 10^5 gain). Range ±300 Volts.
Emission Current	Emission current may be set from 5 to 100 µA.

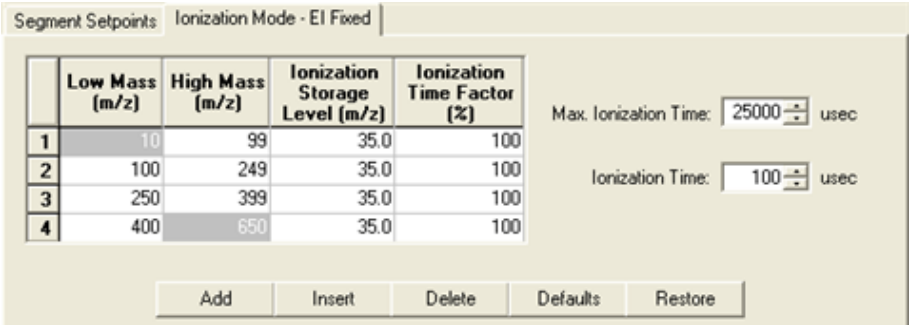
Item	Description
Count Threshold	The minimum number of intensity counts per sampling interval required before a signal is recorded. Values from 0 to 1000 counts; it is typically set to 0 or 1 count.
Mass Defect	Mass defect is defined as the difference between the nominal mass of an atom (or ion) and its exact mass. Values from -300 mu per 100u to +300 mu per 100u can be set.
Cal Gas	Click if using Calibration gas in the Method segment.

Ionization Mode - EI Auto



Item	Description
Mass Range Segment Breaks	Set between 1 and 6 scan segments, each has a contiguous mass-range segment. Overall, the set covers the entire mass range of 10 to 650 m/z. The usere can change only the intermediate segment boundaries.
Ionization Storage Level	Set the rf voltage for during the ionization period. Values from 5 to 150 m/z.
Ionization Time Factor	Set the Ionization Time Factor, A percent, is a number that is multiplied by the calculated ionization time (determined by the AGC pre-scan pulse) to give the actual ionization time. Values from 1 to 999%.
Target TIC Value	Use theTarget TIC value to determine how many ions AGC allows into the ion trap during the calculated ionization time. Range of values is 10 to 65000.
Maximum Ionization Time	Set the limit for the longest ionization time AGC can use. Values from 10 to 65000 μsec.
Prescan Ionization Time	Determine the number of ions formed for the prescan. This value is used to calculate the ionization time for the analytical scan. Range 10 to 2500 usec.
Background Mass	Set the lowest mass for determining the target TIC (total ion current) value; all ions of lower mass are ejected from the ion trap before the AGC prescan pulse. The background mass can be set to any value from 10 m/z to 300 m/z; it is typically set to 45 m/z.
rf Dump Value	Specify the high m/z used for the prescan. It must be as high or higher than the analytical scan range high mass.

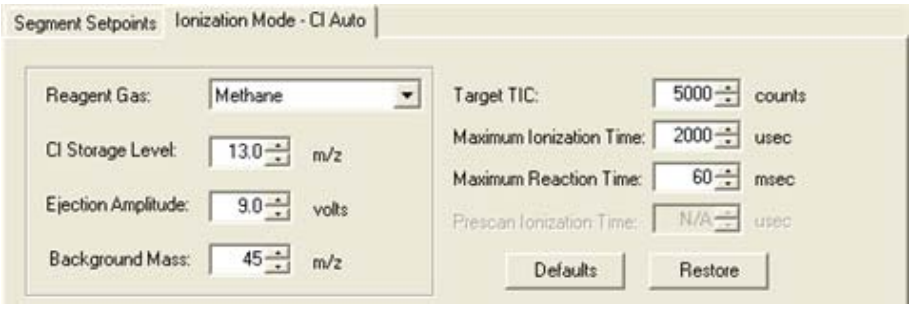
Ionization Mode - EI Fixed



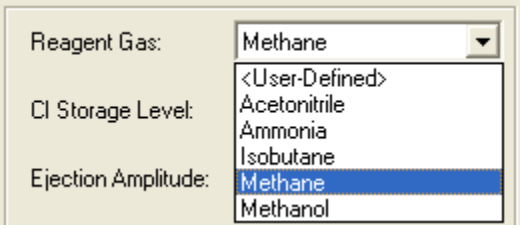
Item	Description
Mass Range Segment Breaks	The EI scan has between 1 and 6 scan segments. Each holds a contiguous mass-range segment. Overall, the set covers the entire mass range of 10 to 650 m/z. The users can change only the intermediate segment boundaries.
Ionization Storage Level	The rf voltage used during the ionization period. Values from 5 to 150 m/z.
Ionization Time Factor	The Ionization Time Factor, given as a percent, is a number that is multiplied by the calculated ionization time (determined by the AGC pre-scan pulse) to give the actual ionization time. Values from 1 to 999%.
Ionization Time	Sets the fixed ionization time. Values from 10 to 65000 μsec.
Max Ionization Time	Sets the maximum ionization time used by the system.

The CI Parameters

CI Auto

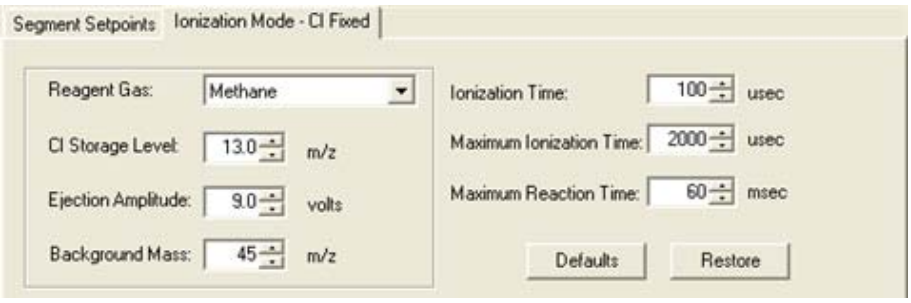


Reagent Gas



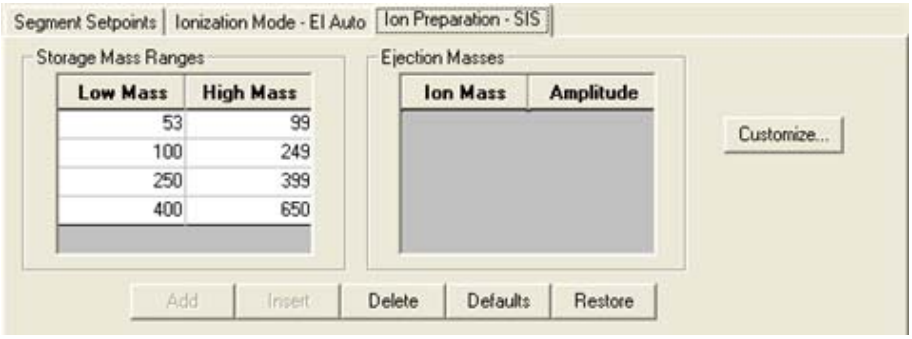
Item	Description
Reagent Gas	Select CI reagent for application. Select User-Defined for gases not listed.
CI Storage level	Value of the smallest mass stored in the ion trap during the ionization and reaction period of the reagent gas. Values from 5 to 150 m/z.
Ejection Amplitude (v)	This voltage actively ejects unwanted ions (i.e., not reagent ions) that are produced during the ionization stage of the CI scan function. When this value is set to 0, active ejection is disabled.
Background mass	The mass value that is greater than or equal to the mass of the largest reagent ion produced by the selected reagent gas. Values from 10 to 300 m/z.
Target TIC Value	Target TIC value determines how many ions are allowed in the ion trap. CI uses a portion of the ions detected during the previous analytical scan to calculate the ionization and reaction times for the next analytical scan. Values from 10 to 30000.
Maximum ionization time	Maximum time that energetic electrons, emitted from the filament, are allowed to interact with reagent gas molecules to form reagent ions. In CI, the maximum ionization time can be set to any value from 10 to 2500 μsec.
Maximum reaction time	Maximum time that reagent gas ions are allowed to react with sample molecules to form ions. The maximum reaction time can be set to any value from 1 to 128 milliseconds.
Prescan Ionization Time	Ionization time of the prescan uses in MS/MS. This is normally set to 200 μsec for CI.

CI Fixed Parameters



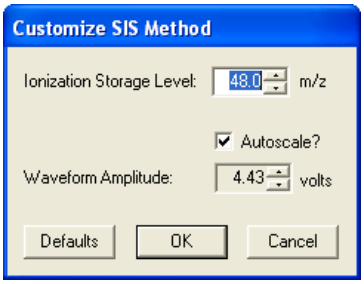
Item	Description
Reagent Gas	Select CI reagent for application. Select User-Defined for gas not listed.
CI Storage level	Value of the smallest mass stored in the ion trap during the ionization and reaction period of the reagent gas. Values from 5 to 150 m/z.
Ejection Amplitude (v)	This voltage actively ejects unwanted ions (i.e., not reagent ions) that are produced during the ionization stage of the CI scan function. When this value is set to 0, active ejection is disabled. Range 0 to 65.0 volts
Background mass	The mass value that is greater than or equal to the mass of the largest reagent ion produced by the selected reagent gas. Values from 10 to 300 m/z.
Ionization Time	Fixed time CI reagent ions are formed. Values from 10 to 2000 usec.
Maximum ionization time	Maximum time that energetic electrons, emitted from the filament, are allowed to interact with reagent gas molecules to form reagent ions. In CI, the maximum ionization time can be set to any value from 10 to 2500 μsec.
Maximum reaction time	Maximum time that reagent gas ions are allowed to react with sample molecules to form ions. The maximum reaction time can be set to any value from 1 to 128 milliseconds.

Ion Storage (SIS) Parameters



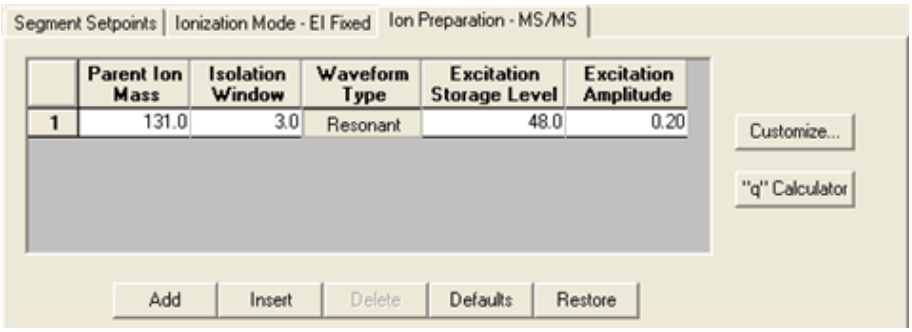
Item	Description
Storage Mass Ranges	Table to enter ion(s) or range of ions for selective storage. Enter up to five mass ranges.
Low Mass	Low m/z integer mass. Mass range from 25 m/z to 650 m/z.
High Mass	High m/z integer mass. Mass range from 25 m/z to 650 m/z.
Ejection Masses	Enter ion(s) for selective ejection. Enter up to five ions.
Ion Mass	Integer mass(es) of those ion(s) to be ejected. Use ADD button to enter value.
Amplitude	Range is 1% to 200% with a default of 100%.

Customize SIS



Item	Description
Ionization Storage Level	Minimum mass that can be stored and isolated. Range: 20 m/z ≤ mass ≤ 60 m/z. Default = 48 m/z.
Autoscale	SIS waveform amplitude is automatically scaled as a function of the frequency components and storage rf voltage selected. By clearing Autoscale, the user can enter a waveform amplitude.

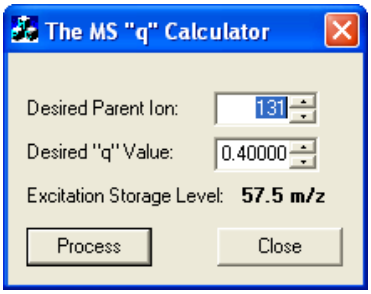
The MS/MS Ion Prep Method



Item	Description
Isolation	Mass to be isolated and window of isolation
Parent Ion Mass (m/z)	Integer or exact mass. Parent ion mass range is 50 to 650 m/z.
Isolation Window (m/z)	Integral and fractional mass isolation windows are both accepted. Range is 1.0 to 7.0 m/z and is mass dependent. The default value is 3.0 m/z.
Dissociation	Waveform type and used for dissociation.
Waveform Type	Nonresonant or resonant excitation.
Excitation Storage Level	Rf storage level in m/z when the dissociation waveform is applied following isolation. The excitation storage level range depends on the percursor mass, but the storage level must be more than 2 mass units below the lowest product ion value.

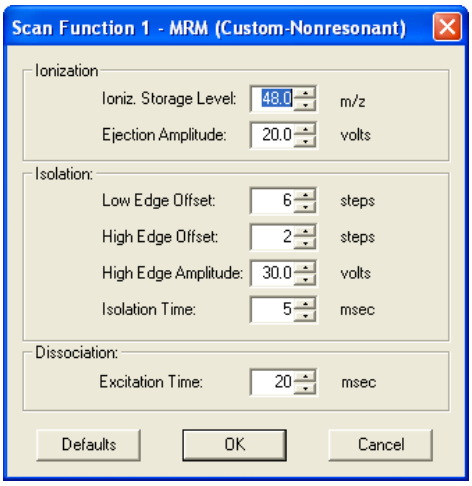
Item	Description
Excitation Amplitude	Range for nonresonant excitation is 0 to 100 volts. For resonant excitation, the range is 0 to 60 volts. Default values for nonresonant excitation is 20 volts and 0.2 volts for resonant excitation.

The MS “q” Calculator



Item	Description
MS q Calculator	Use the q Calculator to calculate suggested excitation storage levels.
Desired Parent Ion	Enter the desired parent ion to determine its optimal corresponding excitation storage level.
Desired q Value	Empirically observed “q” value of 0.4 provides an optimal yield of product ions.

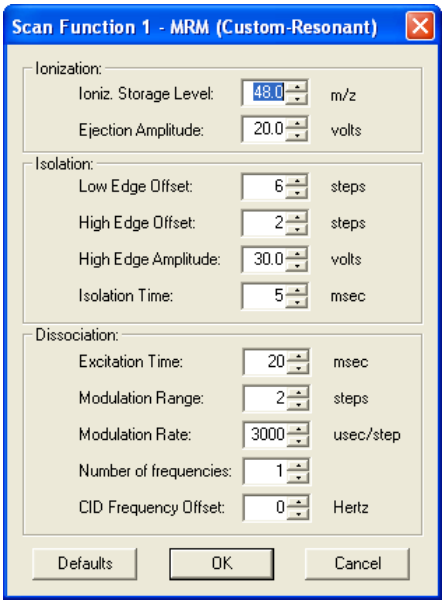
Customize Non-resonant Method



Item	Description
Ionization Storage Level	The m/z value the rf is maintained during ionization and the coarse isolation. Range 35 to 160 m/z (upper limit of range depends on parent ion m/z), default = 48 m/z.

Item	Description
Ejection Amplitude	Amplitude (v) of the ejection waveform during the coarse isolation step. Range 0 to 60 volts, default=20.
Low Edge Offset	Integer value step to optimize the ejection of the mass just below the percursor ion mass. Range is 0 to 20 steps. The default value is 6.
High Edge Offset	The integer value step to optimize the ejection of the mass just above the percursor ion mass. Range is -20 to 20 steps.
High Edge Amplitude	Amplitude of broadband waveform use to eject masses above the isolated percursor ion. Default is 30 volts.
Isolation Time	The dwell time during which the rf field is held constant in the high mass ejection step. Range 1 - 10 msec.
Excitation Time	Time for collision-induced dissociation (CID) by ion excitation. Range 0 to 1000 msec. The default is 20 msec.

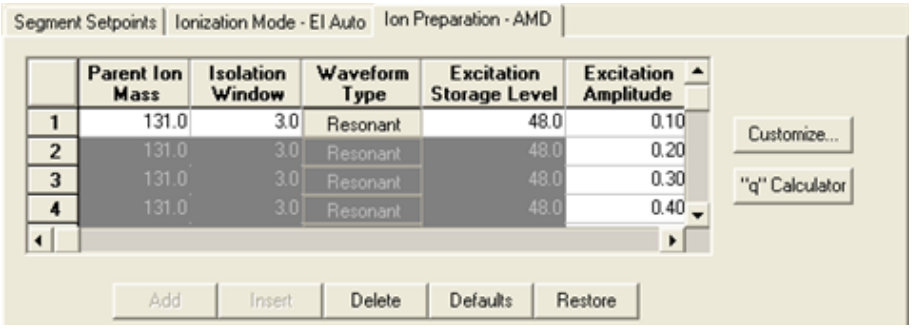
Customize Resonant Method



Item	Description
Ionization Storage Level	The m/z value the rf is maintained during ionization and the coarse isolation. Range 35 to 160 m/z (upper limit of range depends on m/z of the percursor ion), default = 48 m/z.
Ejection Amplitude	Amplitude (v) of the ejection waveform during the coarse isolation step. Range 0 to 60 volts, default=20.
Low Edge Offset	Integer value step to optimize the ejection of the mass just below the percursor ion mass. Range is 0 to 20 steps. The default value is 6.

Item	Description
High Edge Offset	The integer value step to optimize the ejection of the mass just above the percursor ion mass. Range is -20 to 20 steps.
High Edge Amplitude	Amplitude of broadband waveform use to eject masses above the isolated percursor ion. Default is 30 volts.
Isolation Time	The dwell time during which the rf field is held constant in the high mass ejection step. Range 1 - 10 msec.
Excitation Time	Time for collision-induced dissociation (CID) by ion excitation. Range 0 to 1000 msec. The default is 20 msec
Modulation Range	Mass range over which the rf storage field is modulated during resonant CID. The range is 0 to 12 steps, default is 2 steps. Value of 0 gives a fixed rf storage field, i.e., no modulation.
Modulation Rate	The number of microseconds that will be spent at each step. The range is 29 usec to 5600 usec, default is 3000 usec/step.
Number of Frequencies	Enter an odd integer in the range of 1 to 121. A frequency number of one generates a single supplementary frequency applied to the end caps. An integer of 3, generates three frequencies: the resonance frequency and frequencies 500 Hz above and below that frequency.
CID Frequency Offset	To offset the dissociation frequency. The CID frequency can be adjusted between ± 3000 Hz.

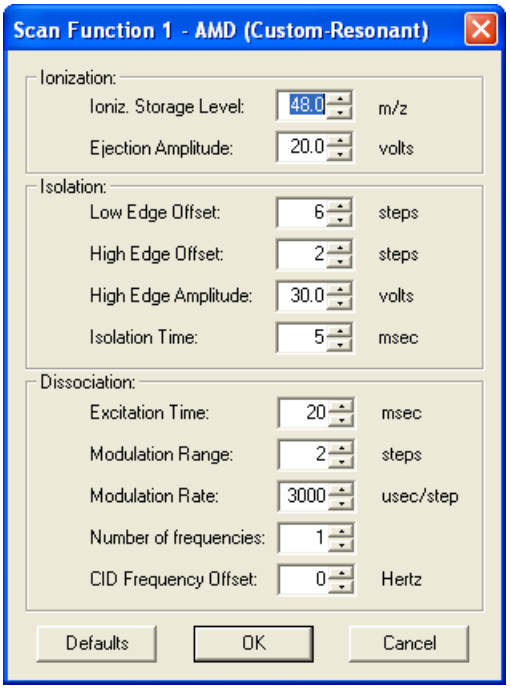
Automated Methods Development (AMD)



Item	Description
Parent Ion Mass (m/z)	Integer or exact mass. Parent ion mass range is 50 to 650 m/z.
Isolation Window (m/z)	Integral and fractional mass isolation windows are both accepted. Range is 1.0 to 14.0 m/z and is mass dependent. The default value is 3.0 m/z.
Waveform Type	Nonresonant or resonant excitation.
Excitation Storage Level	Rf storage level in m/z when the dissociation waveform is applied following isolation. The excitation storage level range depends on the parent mass, but the storage level must lie more than 2 mass units below the lowest product ion value.

Item	Description
Excitation Amplitude	Range for nonresonant excitation is 0 to 100 volts. For resonant excitation, the range is 0 to 60 volts. Default values for nonresonant excitation is 20 volts and 0.2 volts for resonant excitation.

Customize Resonant Method — AMD

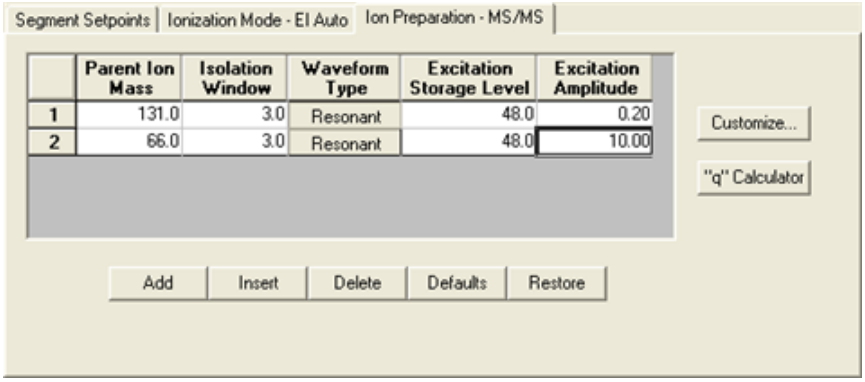


Item	Description
Ionization Storage Level	The m/z value the rf is maintained at during ionization and the coarse isolation. Range 35 to 160 m/z, default = 48 m/z.
Ejection Amplitude	Amplitude (v) of the ejection waveform during the coarse isolation step. Range 0 to 60 volts, default=20.
Low Edge Offset	Integer value step to optimize the ejection of the mass just below the percursor ion mass. Range is 0 to 20 steps. The default value is 6 .
High Edge Offset	The integer value step to optimize the ejection of the mass just above the percursor ion mass. Range is -20 to 20 steps.
High Edge Amplitude	Amplitude of broadband waveform used to eject masses above the isolated percursor ion. Default is 30 volts.
Isolation Time	The dwell time during which the rf field is held constant in the high mass ejection step. Range 1 - 10 msec.

Item	Description
Excitation Time	Time for collision-induced dissociation (CID) by ion excitation. Range 0 to 1000 msec. The default is 20 msec.
Modulation Range	Mass range over which the rf storage field is modulated during resonant CID. The range is 0 to 10 steps, default is 2 steps. Value of 0 gives a fixed rf storage field, i.e., no modulation.
Modulation Rate	The number of microseconds that will be spent at each step. The range is 29 usec to 5600 usec, default is 3000 usec/step.
Number of Frequencies	Enter an odd integer in the range of 1 to 121. A frequency number of one generates a single supplementary frequency applied to the end caps. An integer of 3, generates three frequencies: the resonance frequency and frequencies 500 Hz above and below that frequency.
CID Frequency Offset	To offset the dissociation frequency. The CID frequency can be adjusted between ± 3000 Hz.

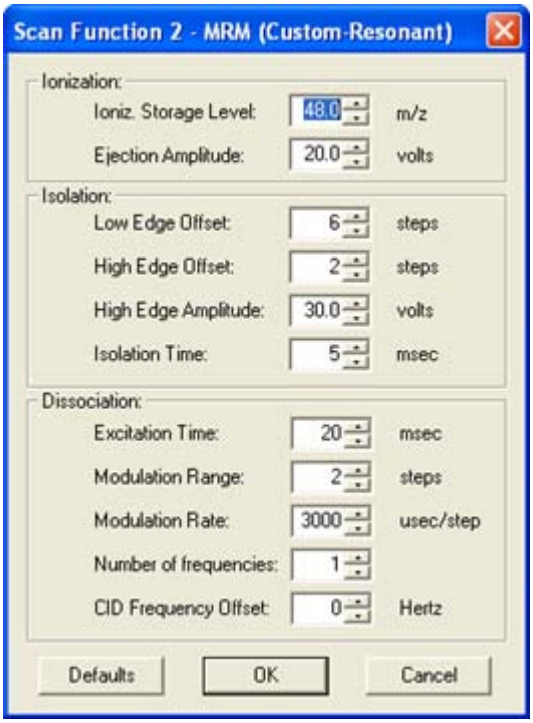
Ion Preparation MS/MS

Set up Multiple Reaction Monitoring by adding lines to a MS/MS run with different percursor ion masses and different dissociation parameters.



Item	Description
Parent Ion Mass (m/z)	Integer or exact mass. Parent ion mass range is 50 to 650 m/z.
Isolation Window (m/z)	Integral and fractional mass isolation windows are both accepted. Range is 1.0 to 14.0 m/z and is mass dependent. The default value is 3.0 m/z.
Waveform Type	Nonresonant or resonant excitation.

Item	Description
Excitation Storage Level	Rf storage level in m/z when the dissociation waveform is applied following isolation. The excitation storage level range depends on the percursor mass, but the storage level must lie more than 2 mass units below the lowest product ion value.
Excitation Amplitude	Range for nonresonant excitation is 0 to 100 volts. For resonant excitation, the range is 0 to 60 volts. Default values for nonresonant excitation is 20 volts and 0.2 volts for resonant excitation.
Ionization Storage Level	The m/z value the rf is maintained at during ionization and the coarse isolation. Range 35 to 160 m/z, default = 48 m/z.



Item	Description
Ejection Amplitude	Amplitude (v) of the ejection waveform during the coarse isolation step. Range 0 to 60 volts, default=20.
Low Edge Offset	Integer value step to optimize the ejection of the mass just below the percursor ion mass. Range is 0 to 20 steps. The default value is 6.
High Edge Offset	The integer value step to optimize the ejection of the mass just above the percursor ion mass. Range is -20 to 20 steps.

Item	Description
High Edge Amplitude	Amplitude of broadband waveform use to eject masses above the isolated percursor ion. Default is 30 volts.
Isolation Time	The dwell time during which the rf field is held constant in the high mass ejection step. Range 1 - 10 msec.
Excitation Time	Time for collision-induced dissociation (CID) by ion excitation. Range 0 to 1000 msec. The default is 20 msec.
Modulation Range	Mass range over which the rf storage field is modulated during resonant CID. The range is 0 to 10 steps, default is 2 steps. Value of 0 gives a fixed rf storage field, i.e., no modulation.
Modulation Rate	The number of microseconds that will be spent at each step. The range is 29 usec to 5600 usec, default is 3000 usec/step.
Number of Frequencies	Enter an odd integer in the range of 1 to 121. A frequency number of one generates a single supplementary frequency applied to the end caps. An integer of 3, generates three frequencies: the resonance frequency and frequencies 500 Hz above and below that frequency.
CID Frequency Offset	To offset the dissociation frequency. The CID frequency can be adjusted between ± 3000 Hz.

MS^n

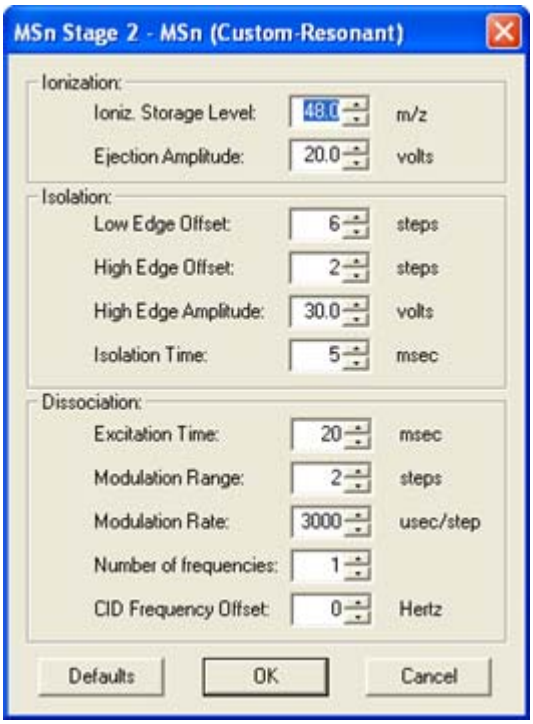
MS^n uses two parent ions for sequential dissociation. The additional dissociation step can be used to increase selectivity of analyte versus background or for additional structure information.

First, work out optimized conditions for MS/MS of the first parent ion. AMD will make this process go faster.

Then optimize the conditions for dissociation of that product ion (entered under parent ion 2). You may need to make sequential injections using the MS^n method. If the second generation product ion is in the original EI or CI spectrum, then you can use AMD to find the optimum conditions.

Item	Description
Parent Ion Mass (m/z)	Integer or exact mass. Parent ion 1 mass range is 50 to 650 m/z. Parent ion 2 mass range is from 50 to (parent ion-1)m/z, and so on.

Item	Description
Isolation Window (m/z)	Integral and fractional mass isolation windows are both accepted. Range is 1.0 to 14.0 m/z and is mass dependent. The default value is 3.0 m/z.
Waveform Type	Nonresonant or resonant excitation.
Excitation Storage Level	Rf storage level in m/z when the dissociation waveform is applied following isolation. The excitation storage level range depends on the parent mass, but the storage level must lie more than 2 mass units below the lowest product ion value.
Excitation Amplitude	Range for nonresonant excitation is 0 to 100 volts. For resonant excitation, the range is 0 to 60 volts. Default values for nonresonant excitation is 20 volts and 0.2 volts for resonant excitation.



Item	Description
Ionization Storage Level	The m/z value the rf is maintained at during ionization and the coarse isolation. Range 35 to 160 m/z, default = 48 m/z.
Ejection Amplitude	Amplitude (v) of the ejection waveform during the coarse isolation step. Range 0 to 60 volts, default=20.
Low Edge Offset	Integer value step to optimize the ejection of the mass just below the parent ion mass. Range is 0 to 20 steps. The default value is 6 .

Item	Description
High Edge Offset	The integer value step to optimize the ejection of the mass just above the parent ion mass. Range is -20 to 20 steps.
High Edge Amplitude	Amplitude of broadband waveform use to eject masses above the isolated parent ion. Default is 30 volts.
Isolation Time	The dwell time during which the rf field is held constant in the high mass ejection step. Range 1 - 10 msec.
Excitation Time	Time for collision-induced dissociation (CID) by ion excitation. Range 0 to 1000 msec. The default is 20 msec.
Modulation Range	Mass range over which the rf storage field is modulated during resonant CID. The range is 0 to 10 steps, default is 2 steps. Value of 0 gives a fixed rf storage field, i.e., no modulation.
Modulation Rate	The number of microseconds that will be spent at each step. The range 29 usec to 5600 usec, default is 3000 usec/step.
Number of Frequencies	Enter an odd integer in range of 1 to 121. A frequency number of one generates a single supplementary frequency applied to the end caps. An integer of 3, generates three frequencies: the resonance frequency and frequencies 500 Hz above and below that frequency.
CID Frequency Offset	To offset the dissociation frequency. The CID frequency can be adjusted between ± 3000 Hz.

450-GC Method Command Reference

450-GC AutoSampler

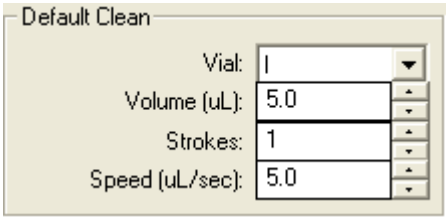
When the 8400 AutoSampler or 8410 AutoInjector is selected, the AutoSampler window may contain up to five sections. The topmost section is common to all modes of operation.

In addition, all modes of operation also include a Default Clean section and a Clean Mode section. When Viscous, Volatile, or User Defined modes are selected, the Internal Standard section is displayed. In User Defined mode, the More User Defined button is displayed to provide access to the dialog box to set the User Defined parameter. The Default Settings for Predefined AutoSampler Modes contains a table showing the parameters that are used by the 8400/8410 for each of the predefined modes of operation.

Item	Description
AutoSampler Type	8400, 8410, or None Specifies whether or not an 8400 AutoSampler or 8410 AutoInjector is installed on the 450-GC. If an 8400 or 8410 is not installed on the GC or is turned off, select None. When 8400 or 8410 is selected, the following items are displayed for editing.
Syringe Size (uL)	1, 2, 5, 10, 50, 100, or 250 uL Selects the size of the syringe that is installed on the 8400/8410 for use with this method.
Agitation Strokes (SPME mode only)	0 to 500,000 Specifies the number of mixing strokes of the cleaning solvent.
Injection Mode	Std Split/Splitless, Std On Column, Neat, Viscous, Volatile, SPME mode, or User Defined Sets the 8400/8410 parameters for the predefined modes of operation.
Adsorb Time (min) (SPME mode only)	0 to 999.99 minutes Specifies the time that the sample is in the in the vial.
Desorb Time (min) (SPME mode only)	0 to 999.99 minutes Specifies the time that sample is in the injector.

Item	Description
Sample Depth (%)	0 to 100 % Specifies how far the syringe needle is to go down into the sample vial. 100% is the bottom of the vial. 0% is the bottom of the vial septum.
Solvent Depth (%)	0 to 100 % Specifies how far the syringe needle is to go down into the solvent vial. 100% is the bottom of the vial. 0% is the bottom of the vial septum.

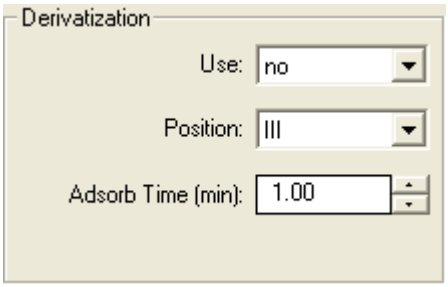
Default Clean Section



To ensure Default Cleaning occurs press one of the following: the Stop button on the front panel of the 450-GC, the Reset button on the 450-GC Status Window in Workstation System Control, or the Stop Automation menu item in the Workstation System Control Automation menu. Default Cleaning occurs if 8400/8410 has been interrupted or a fault has occurred casing the AutoSampler to abort its regularly programmed sequence of events.

Item	Description
Vial	I, II, or III Specifies which of the three solvent vials will be used by Default Cleaning
Volume (uL)	0 to 10.0 microliters with 10 uL syringe 0 to 5.0 microliters with 5 uL syringe Specifies the amount of cleaning solvent that will be drawn up with each syringe cleaning stroke.
Strokes	0 to 10 Specifies the number of times the cleaning solvent will be drawn up into the syringe and expelled into the waste cup.
Speed (uL/sec)	0.1 to 50.0 microliter per second with 10 microliter syringe 0.1 to 25.0 microliter per second with 5 microliter syringe Specifies the speed at which the cleaning solvent will be drawn up into the syringe and the speed at which it is expelled into the waste cup.

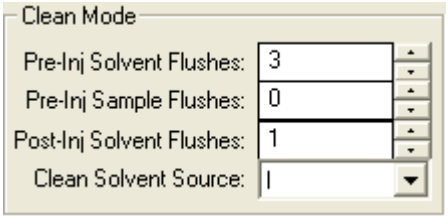
Derivatization



NOTE: SPME mode only

Item	Description
Use	Yes or No Specifies whether or not derivatization is used.
Position	I, II, or III Specifies which of the three solvent vials will be used by Default Cleaning
Adsorb Time (min.)	0 to 999.99 Specifies the length of time for derivatization

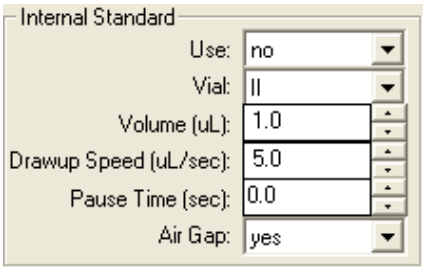
Clean Mode Section



Item	Description
Pre-Inj Solvent Strokes (SPME mode only)	0 to 99 Specifies number of mixing strokes before autosampler progresses to sampling (adsorb) step.
Post-Inj Solvent Strokes (SPME mode only)	0 to 99 Specifies number of mixing strokes after autosampler has desorbed sample
Pre-Inj Solvent Flushes	0 to 99 Specifies the number of times each selected cleaning solvent will be drawn up into the syringe and expelled into the waste cup before flushing with next cleaning solvent (if more than one cleaning solvent source is specified) or the sample.
Pre-Inj Sample Flushes	0 to 99 Specifies the number of times the sample will be drawn up into the syringe and expelled into the waste cup before the syringe is loaded for injection.

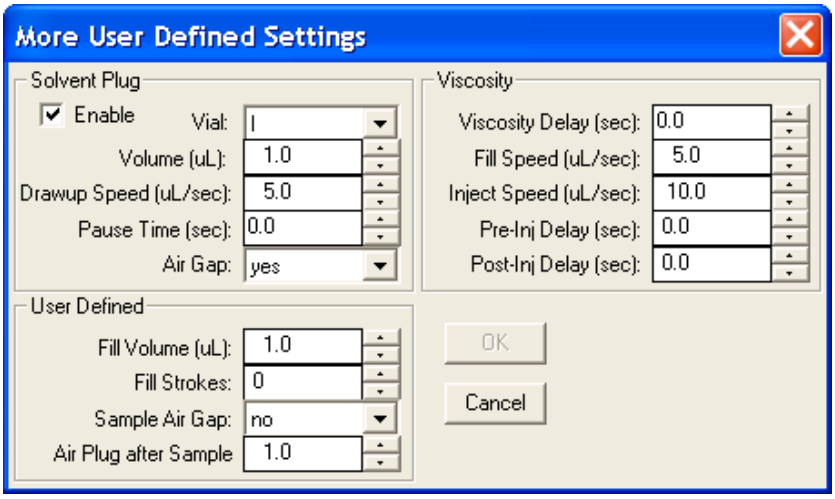
Item	Description
Post-Inj Solvent Flushes	0 to 99 Specifies the number of times each selected cleaning solvent will be drawn up into the syringe and expelled into the waste cup before flushing with next cleaning solvent (if more than one cleaning solvent source is specified).
Clean Solvent Source	I, II, III, I & II, I & III, II & III, or I & II & III Selects which solvent vial or sequence of solvent vials will be used to flush the syringe before and after injection.
Adsorb Time (min.) (SPME mode only)	0 to 999.99 Specifies the time cleaning solvent is in the in the vial.
Desorb Time (min.) (SPME mode only)	0 to 999.99 Specifies the time cleaning solvent is in the injector.

Internal Standard Section



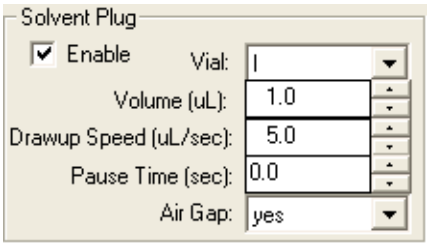
Item	Description
Use	Yes or No If Yes, an internal standard addition will be used. When internal standard addition is used, the internal standard solution will be drawn up into the syringe from the specified solvent vial before the sample is drawn up.
Vial	I, II, or III Selects which solvent vial contains the internal standard.
Volume (uL)	0 to 9.0 microliter with 10 microliter syringe 0 to 4.9 microliter with 5 microliter syringe Specifies the amount of internal standard to be drawn into the syringe before the sample.
Drawup Speed (uL/sec)	0.1 to 50.0 microliter per second with 10 microliter syringe 0.1 to 25.0 microliter per second with 5 microliter syringe Specifies the speed at which the internal standard will be drawn up into the syringe.
Pause Time (sec)	0 to 9.9 seconds Specifies how long the syringe is to remain in the internal standard vial after drawing up the internal standard.
Air Gap	Yes or No If Yes, 1 microliter of room air will be drawn into the syringe to create an air gap between the internal standard and the sample.

More User Defined Settings Dialog Box



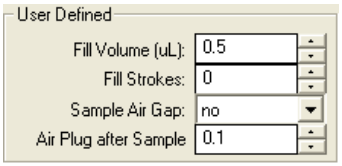
This dialog box is accessed from “More User Defined…” button that is displayed when the User Defined mode is selected.

Solvent Plug Settings



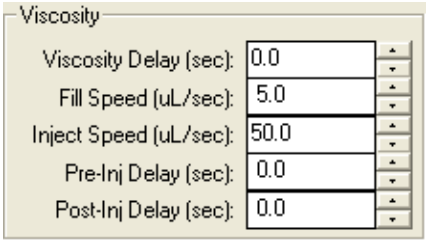
Item	Description
Enable (checkbox)	Specifies whether or not a solvent plug is used. When the checkbox is unchecked, all the fields in the Solvent plug section are disabled and grayed out.
Vial	I, II, or III Selects which solvent vial to use for the solvent plug.
Volume (uL)	0 to 10.0 microliter with 10 microliter syringe 0 to 5.0 microliter with 5 microliter syringe Specifies the amount of solvent to be drawn into the syringe before the sample or internal standard.
Drawup Speed (uL/sec)	0.1 to 50.0 microliter per second with 10 microliter syringe 0.1 to 25.0 microliter per second with 5 microliter syringe Specifies the speed at which the solvent will be drawn up into the syringe.
Pause Time (sec)	0 to 9.9 seconds Specifies how long the syringe is to remain in the solvent vial after drawing up the solvent.
Air Gap	Yes or No If Yes, 1 microliter of room air will be drawn into the syringe to create an air gap before the solvent plug.

User Defined Settings



Item	Description
Fill Volume (uL)	0 to 10.0 microliter with 10 microliter syringe 0 to 5.0 microliter with 5 microliter syringe Specifies the sample volume that will be used for each fill stroke.
Fill Strokes	0 to 99 Specifies the number of the times the sample will be “pumped” in and out of the syringe before loading the sample volume into the syringe.
Sample Air Gap	Yes or No If Yes, 1 microliter of room air will be drawn into the syringe to create an air gap before the sample plug.
Air Plug after Sample	0 to 10.0 microliter with 10 microliter syringe 0 to 5.0 microliter with 5 microliter syringe Specifies the volume of room air that will be drawn into the syringe after it is loaded with sample.

Viscosity Settings



Item	Description
Viscosity Delay (sec)	0 to 9.9 seconds Specifies how long the syringe is to remain in the sample vial after drawing up the sample.
Fill Speed (uL/sec)	0.1 to 50.0 microliter per second with 10 microliter syringe 0.1 to 25.0 microliter per second with 5 microliter syringe Specifies the speed at which the sample will be drawn up into the syringe.
Inject Speed (uL/sec)	0.1 to 50.0 microliter per second with 10 microliter syringe 0.1 to 25.0 microliter per second with 5 microliter syringe Specifies the speed at which the contents of the syringe will be expelled into the injector.
Pre-Inj Delay (sec)	0 to 99.9 seconds Specifies the length of time the syringe needle resides in the injector before expelling the syringe contents.

Item	Description
Post-Inj Delay (sec)	0 to 99.9 seconds Specifies the length of time the syringe needle remains in the injector after expelling the syringe contents.

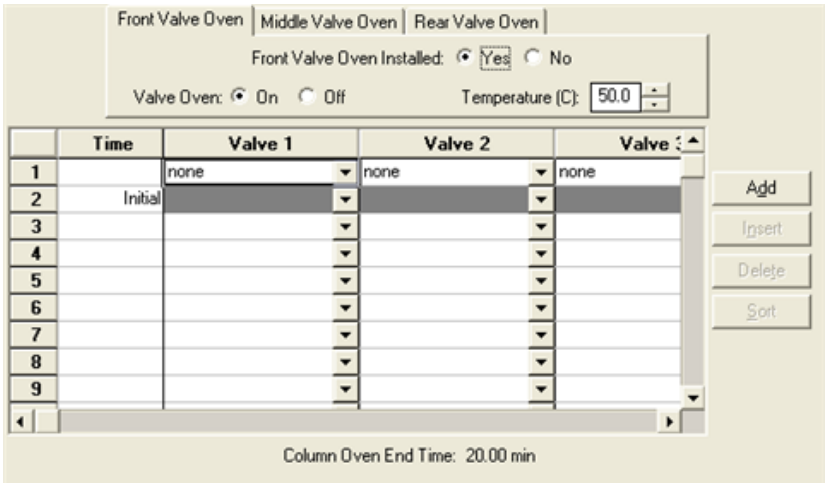
Default Settings for Predefined AutoSampler Modes

The following table lists the parameter settings used for each of the Predefined 8400/8410 modes using a 10 microliter syringe. If the predefined modes do not work acceptably for your samples, use the User Defined mode to enter settings that will work better with your samples. The values listed in this table provide a starting point for setting the various parameters.

Parameter	Std Split/ Splitless	Std On-Column	Neat ⊕	Volatile	Viscous
Solvent Plug Settings:	Solvent plug is not used with predefined modes. If you wish to use solvent plug injections, use User Defined mode.				
PreDefined Settings:					
Fill Volume	7.5 µL	7.5 µL	Not used	Not used	Not used
Fill Strokes	5	5	0 ⊕	0	0
Sample Air Gap	No	No	No	No	No
Air Plug after Sample	1 µL	1 µL	1 µL	1 µL	1 µL
Viscosity Settings:					
Viscosity Delay	0 sec	0 sec	0 sec	6 sec	9.9 sec
Fill Speed	2 µL /sec	2 µL /sec	2 µL /sec	1 µL /sec	1 µL /sec
Inject Speed	50 µL /sec	2 µL /sec	50 µL /sec	1 µL /sec	5 µL /sec
Pre-Inj Delay	0 sec	0 sec	0 sec	0 sec	0 sec
Post-Inj Delay	0 sec	6 sec	0 sec	0 sec	12 sec

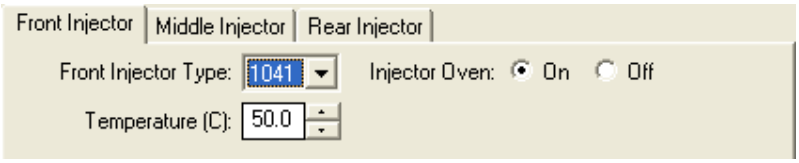
⊕ Instead of fill strokes Neat mode fills the syringe with sample at 2 microliter/sec then expels it into the waste cup at 50 microliter/sec. It does this a total of six times. Then it fills the syringe with sample at 2 microliter/sec and expels it back into the sample vial at 50 microliter/sec. This “pumping” action is done three times. After this is completed, the sample is loaded into the syringe and injected using the parameters in the table.

450-GC Sample Delivery



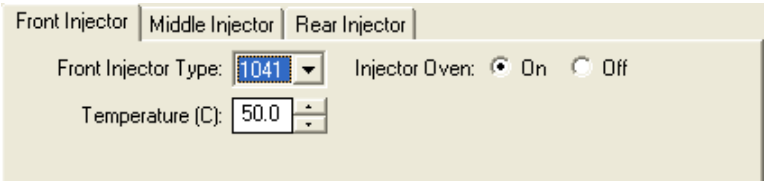
Item	Description
Front Valve Oven Middle Valve Oven Rear Valve Oven	The 450-GC can have up to three valve ovens installed (front, middle, and rear). The tabs at the top of the window select the valve oven position.
Valve Oven Installed	Indicate if the Valve Oven is.
Valve Oven on/off	Indicate if you will use the installed Valve Oven.
Temperature (C)	Specifies the isothermal temperature of each Valve Oven.
Time	Time settings to program how each valve is used initially and at the indicated time.
Valve 1-7	Use the first row to indicate how each valve is used. Click the arrow in the top of each Valve column, and select from the choices displayed in the combo box. The second row contains the initial setting for each Valve when the Method is activated. The following rows contain the time-programmed settings for each of the seven Valves.
Add	Adds a line to the spreadsheet.
Insert	Inserts a line above the currently selected row in the spreadsheet.
Delete	Deletes the currently selected row(s) in the spreadsheet.
Sort	Sorts the spreadsheet rows by time.

450-GC Injector



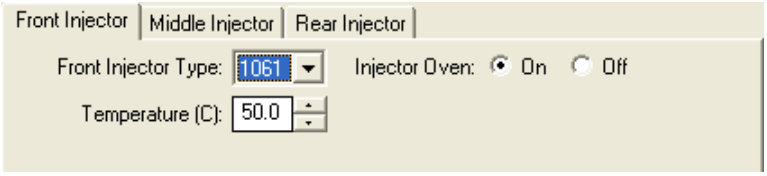
Item	Description
Front Injector Middle Injector Rear Injector	The 450-GC can have up to three injectors installed (front, middle, and rear). The tabs at the top of the window select the injector position.
Injector Type	1041, 1061, 1079, SPT. Specifies the type of injector installed. Select “None” if no injector is installed at that position.
Injector Oven	On or off: Turns the injector oven on or off.

1041 Injector



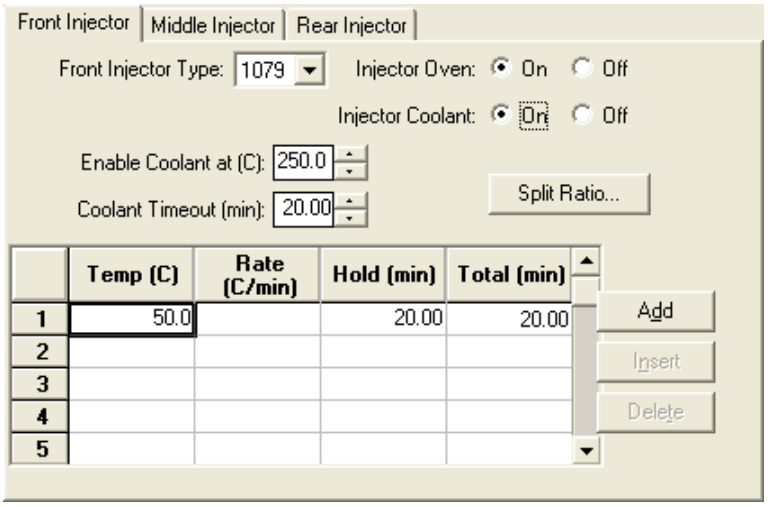
Item	Description
Injector Oven	On or off: Turns the 1041 injector oven on or off.
Temperature (C)	50-450 C: Specifies the oven temperature.

1061 Injector



Item	Description
Injector Oven	On or off: Turns the 1041 injector oven on or off.
Temperature (C)	50-450 ºC: Specifies the oven temperature.

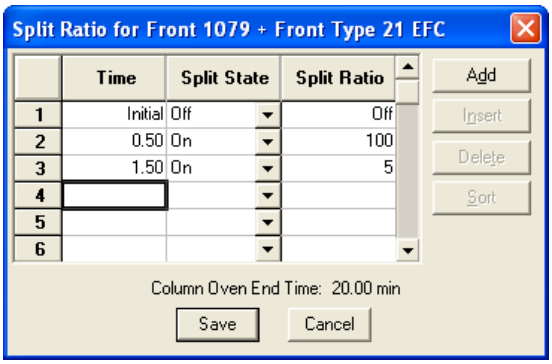
1079 Injector



Item	Description
Injector Coolant	On or Off Turns the coolant valve on when the injector is cooling down. The Coolant valve will not be used if the Off position is selected.
Enable Coolant at (C)	30-450 ºC Specifies the temperature for the coolant valve to turns on.
Coolant Timeout (min)	0.01-999.99 min Provides a safety measure to save coolant after the specified time, if either the injector fails to reach its set temperature or the GC does not go into run.
Split Ratio…	If the appropriate EFC type has been configured, displays the Split Ratio dialog box.
Temp (C)	-99-450 ºC
Rate (C/min)	1-200 ºC /min The Rate in the first row is always blank and cannot be edited.
Hold (min)	0.01-999.99 min
Total (min)	0.01-999.99 min Cannot be edited.
Add	Adds a line to the spreadsheet.
Insert	Inserts a line above the currently selected row in the spreadsheet.
Delete	Deletes the currently selected row(s) in the spreadsheet.

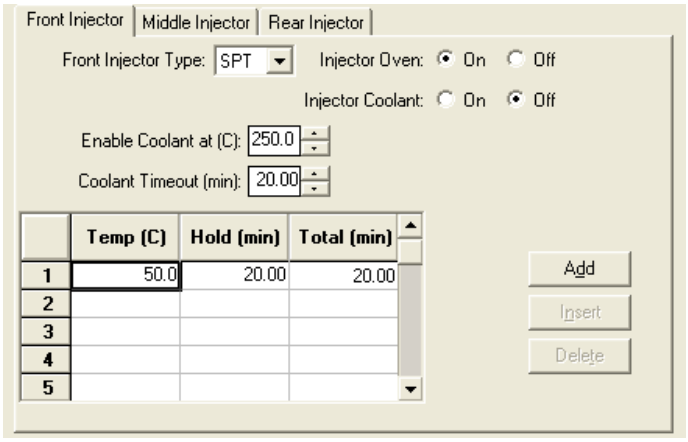
Spilt Ratio Dialog Box

This dialog is displayed from the 450-GC Injector window when a 1079 injector is configured with type 21 EFC.



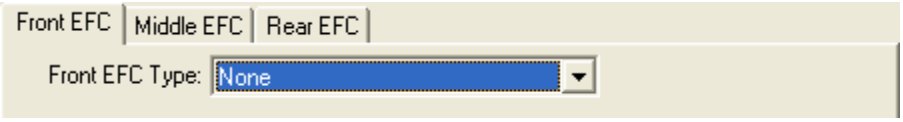
Item	Description
Time	0.00-999.99 min
Split State	On/Off If the split state is ON, then the sample is split according to the split ratio specified. If the split state is OFF, then all the sample enters the column.
Split Ratio	Off, 1 to 10,000 Use a split ratio of 100 after injection to vent the injector. Use a very low split ratio after flushing to conserve carrier gas.
Add	Adds a line to the spreadsheet.
Insert	Inserts a line above the currently selected row in the spreadsheet.
Delete	Deletes the currently selected row(s) in the spreadsheet.
Sort	Sorts the spreadsheet rows by time.

SPT



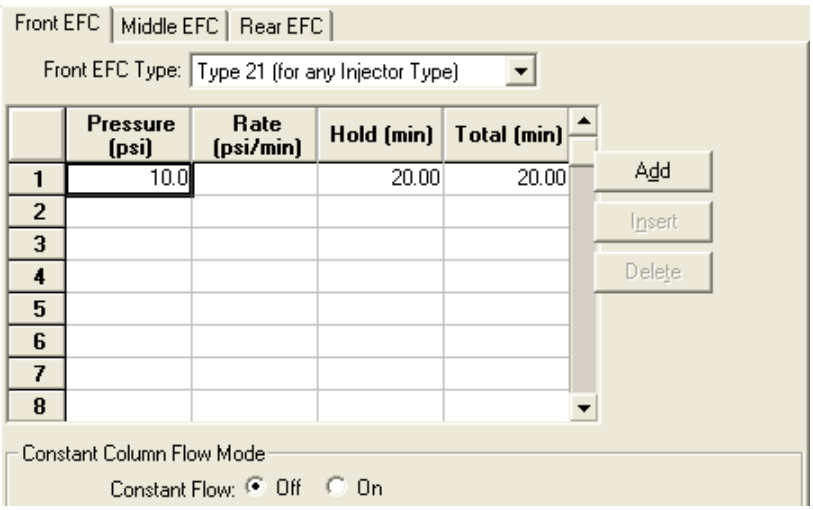
Item	Description
Injector Coolant	On or Off Turns the coolant valve on when the SPT injection device is cooling down. The cryogenic will not be used if the Off position is selected.
Enable Coolant at (C)	30-450 ºC Specifies the temperature for the coolant valve to turns on.
Coolant Timeout (min)	0.01-999.99 min Safety measure to save coolant after the specified time if either the SPT fails to reach its set temperature or the GC does not go into run.
Temp (C)	-185-450 ºC
Hold (min)	0.01-999.99 min
Total (min)	0.01-999.99 min Cannot be edited.
Add	Adds a line to the spreadsheet.
Insert	Inserts a line above the currently selected row in the spreadsheet.
Delete	Deletes the currently selected row(s) in the spreadsheet.

450-GC Flow/Pressure



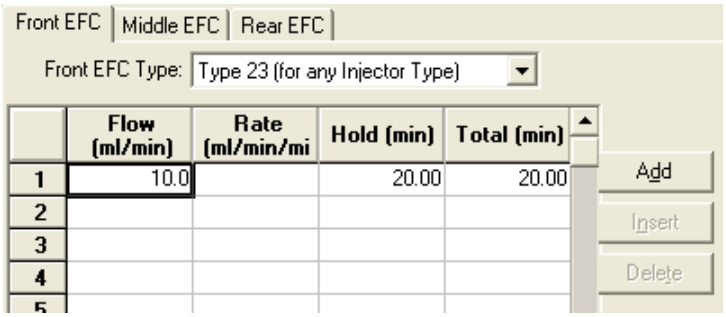
Item	Description
Front EFC Middle EFC Rear EFC	The 450-GC can have up to three injector EFC modules installed (front, middle, and rear). The tabs at the top of the window select the EFC position.
EFC Type	The choices are None, Type 21 or Type 25 (for 1079 injectors), Type 23 (for 1041/1061 injectors), Type 24 (for valved systems). Specifies the type of EFC installed in the selected position.

Type 21 or Type 25 (for 1079 Injectors)



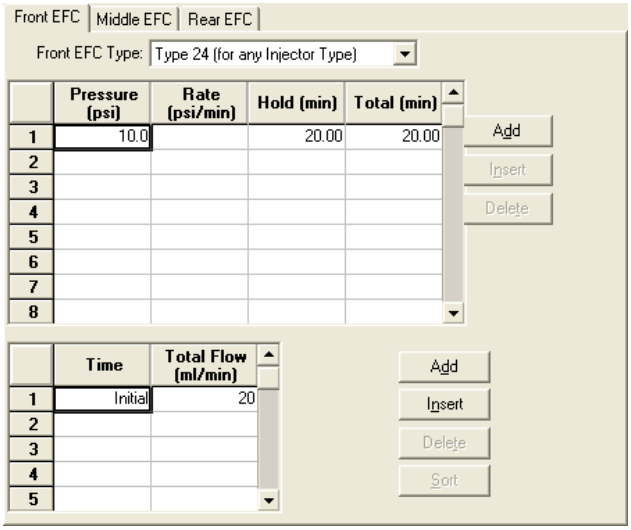
Item	Description
Pressure (psi)	0.1-150.0 psi
Rate (psi/min)	0.01- 400.00 psi/min The Rate in the first row is always blank and cannot be edited.
Hold (min)	0.01- 999.99 min.
Total (min)	0.01-999.99 min Cannot be edited.
Constant Flow	On or offClick Constant flow to disable the spreadsheet and show the constant flow rate value.
Column Flow (ml/min)	Specify the desired constant Column Flow.
Add	Add a line to the spreadsheet.
Insert	Insert a line above the currently selected row in the spreadsheet.
Delete	Delete the currently selected row(s) in the spreadsheet.

Type 23 (for 1041/1061 Injectors)



Item	Description
Flow (ml/min)	0.1- 100.0 ml/min
Rate (ml/min/min)	10.0 ml/min/min The Rate in the first row is always blank and cannot be edited.
Hold (min)	0.01-999.99 min
Total (min)	0.01-999.99 min Cannot be edited.
Add	Add a line to the spreadsheet.
Insert	Insert a line above the currently selected row in the spreadsheet.
Delete	Delete the currently selected row(s) in the spreadsheet.

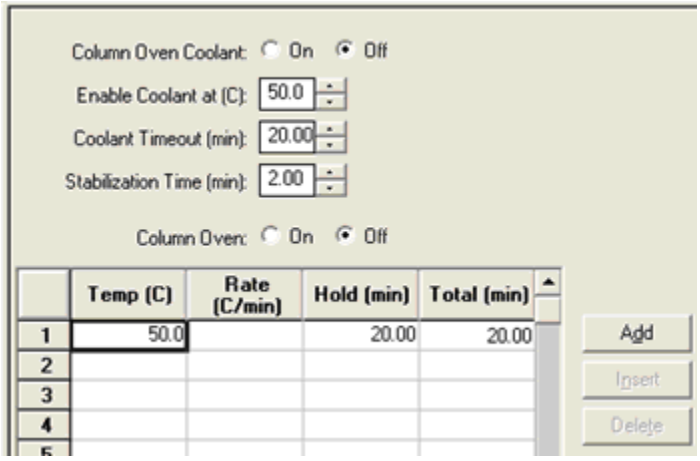
Type 24 (for Valved Systems)



Item	Description
Pressure (psi)	0.1 - 150.0 psi
Rate (psi/min)	0.01-100.0 psi/min The Rate in the first row is always blank and cannot be edited.
Hold (min)	999.99 min

Item	Description
Time	Flow spreadsheet Initial - 999.99 min
Total Flow (ml/min)	1-1000 ml/min.
Add	Add a line to the spreadsheet. This button appears next to both the top and bottom spreadsheet.
Insert	Insert a line above the currently selected row in the spreadsheet. This button appears next to both the top and bottom spreadsheet.
Delete	Delete the currently selected row(s) in the spreadsheet. This button appears next to both the top and bottom spreadsheet.
Sort	Sort the spreadsheet rows by time. This button appears next to the bottom spreadsheet.

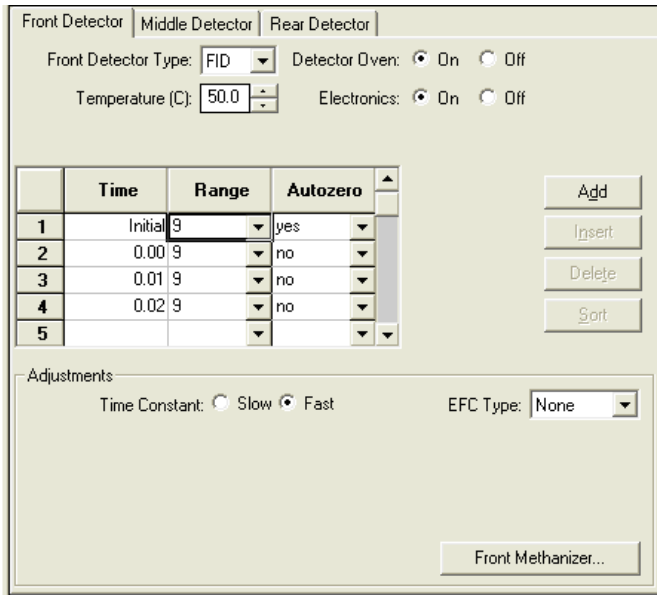
450-GC Column Oven



Item	Description
Column Oven Coolant	On or Off. Specifies whether or not the column coolant will be used.
Enable Coolant at (C)	30- 450 ºC Specifies the temperature at which to enable the coolant.
Coolant Timeout (min)	0.01-999.99 min Provides a safety measure to save coolant after the specified time, if either the injector fails to reach its set temperature or the GC does not go into run.
Stabilization Time (min)	10.0 min Specifies the column Stabilization Time.
Temp (C)	-99 - 450 ºC
Rate (C/min)	0.01- 100.0 ºC/min The Rate in the first row is always blank and cannot be edited.

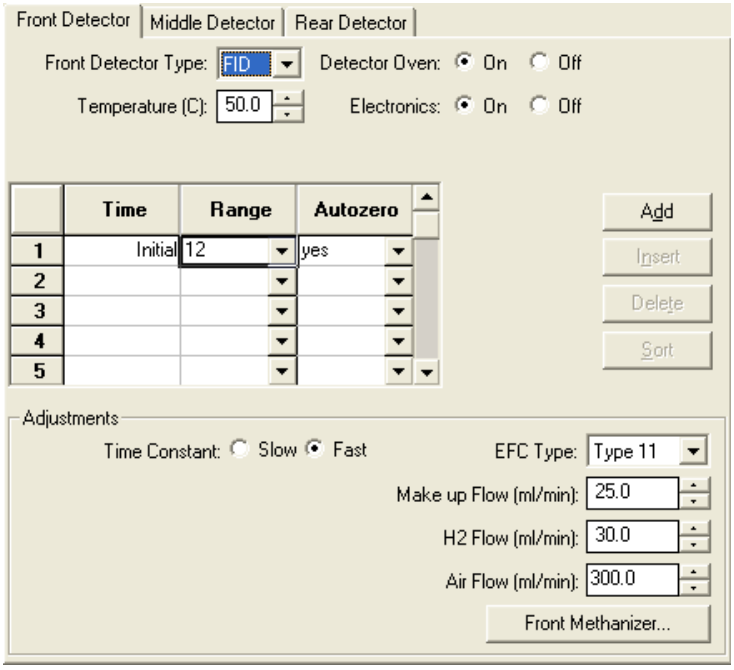
Item	Description
Hold (min)	0.01-999.99 min
Total (min)	0.01-999.99 min Cannot be edited. Column Oven End Time (Total) is displayed in all time-programmed windows of the Method.
Insert	Inserts a line above the currently selected row in the spreadsheet.
Delete	Deletes the currently selected row(s) in the spreadsheet.

450-GC Detector



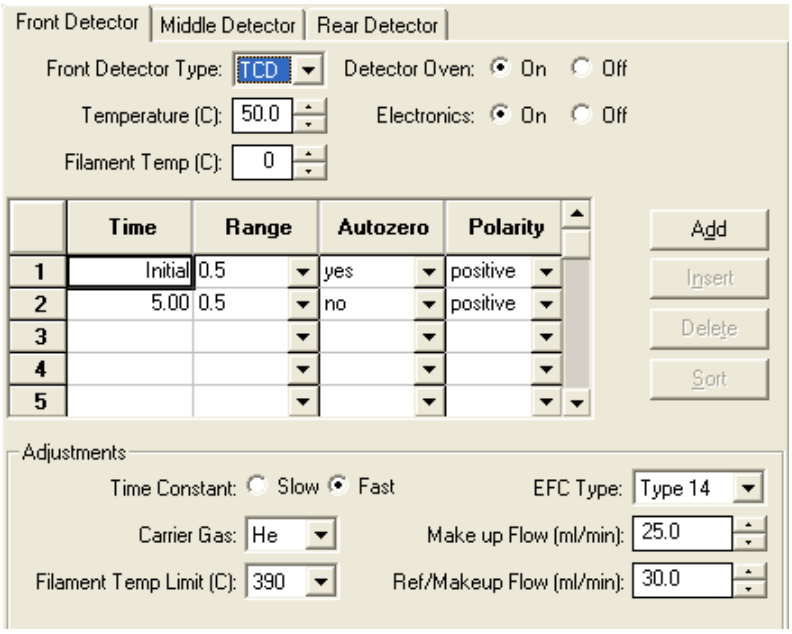
Item	Description
Front Detector Middle Detector Rear Detector	The 450-GC can have up to three detectors installed (front, middle, and rear). The tabs at the top of the window select the detector position.
Detector Type	None, FID, TCD, TSD, ECD, PFPD Specifies the type of detector installed in the selected position.
Detector Oven	On or off. Turns the detector oven on or off.
Electronics	On or off.
Temperature (C)	50- 450 C
Methanizer…	Displays the Methanizer dialog box for the selected position.

FID Detector



Item	Description
Detector Oven	On or off. Turns the detector oven on or off.
Electronics	On or Off. Indicates whether the installed FID will be used or not.
Temperature (C)	50- 450 °C.
Time	Initial - 999.99 min.
Range	9, 10, 11, 12.
Autozero	Yes or No. Set to yes at initial time means that the FID Autozero is on continuous before the run starts.
Add	Adds a line to the spreadsheet.
Insert	Inserts a line above the currently selected row in the spreadsheet.
Delete	Deletes the currently selected row(s) in the spreadsheet.
Sort	Sorts the spreadsheet rows by time.
Time Constant	Slow or Fast.
EFC Type	None or Type 11 for the FID detector.
Make up Flow (ml/min)	0-50 ml/min.
H2 Flow (ml/min)	0-50 ml/min.
Air Flow (ml/min)	0-500 ml/min.
Methanizer Installed	Yes or No.
Methanizer Oven	On or Off.
Temperature (C)	50- 450 C.

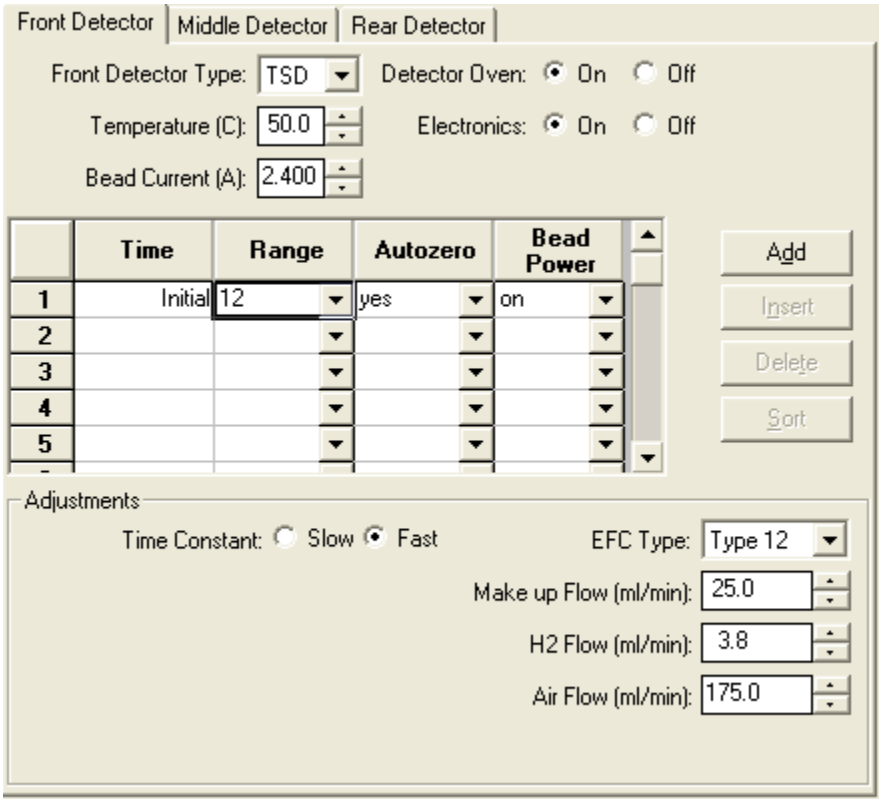
TCD Detector



Item	Description
Detector Oven	On or Off. Turns the TCD oven on or off.
Electronics	On or Off. Indicates if the installed TDC is used.
Temperature (C)	50- 450 °C. Specifies the TCD Temperature.
Filament Temp (C)	0-390 °C. Specifies the Filament Temperature.
Time	Initial - 999.99 min.
Range	0.5 and 5.0 mV. Whenever possible, operate the TCD at the lowest practical filament current.
Autozero	Yes or No. Set to yes at initial time means that the FID Autozero is on continuous before the run starts. Autozero is automatically disabled once the run starts.
Polarity	Positive or Negative. Converts the polarity to reverse the peaks that appear in the negative direction.
Time	Initial - 999.99 min.
Add	Adds a line to the spreadsheet.
Insert	Inserts a line above the currently selected row in the spreadsheet.
Delete	Deletes the currently selected row(s) in the spreadsheet.
Sort	Sorts the spreadsheet rows by time.
Time Constant	Slow or Fast.

Item	Description
Carrier Gas	He or N2/Argon.
Filament Temp Limit (C)	390 or 490 C.
EFC Type	None, Type 13, Type 14 , Type 16. Specifies the installed type.
Make up Flow (ml/min)	0-50 ml/min.
Ref/Makeup Flow (ml/min)	0-100 l/min.
Methanizer Installed	Yes or No.
Methanizer Oven	On or Off.
Temperature (°C)	450 °C.

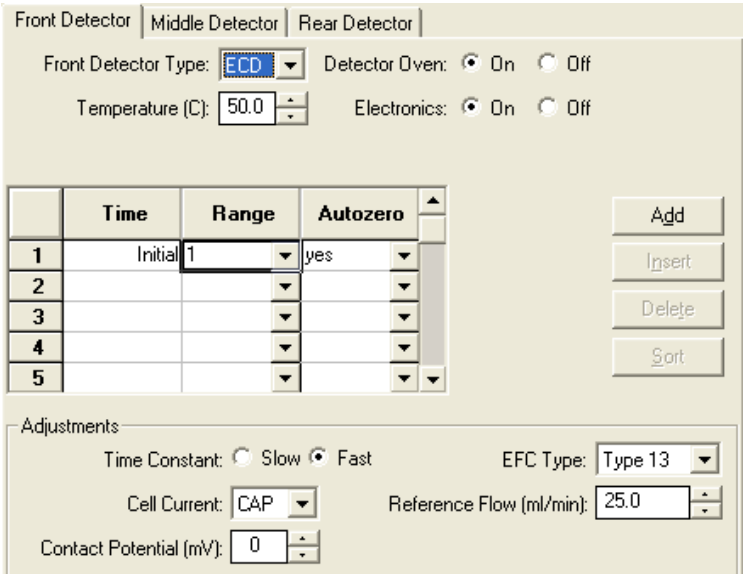
TSD Detector



Item	Description
Detector Oven	On or Off. Turns the detector oven on or off.
Temperature (°C)	50- 450 °C. Specifies the TSD temperature.
Bead Current (A)	2.4 - 3.8 A.
Time	Initial - 999.99 min.
Range	9, 10, 11, 12.

Item	Description
Autozero	Yes or No. Yes at initial time: the TSD Autozero is on continuous before the run starts. Autozero is automatically disabled once the run starts.
Bead Power	On or Off.
Time Constant	Slow or Fast.
Add	Adds a line to the spreadsheet.
Insert	Inserts a line above the currently selected row in the spreadsheet.
Delete	Deletes the currently selected row(s) in the spreadsheet.
Sort	Sorts the spreadsheet rows by time.
EFC Type	None or Type 12 for the TSD detector.
Make up Flow (ml/min)	0-50 ml/min.
H2 Flow (ml/min)	0-6.0 ml/min.
Air Flow (ml/min)	0- 200 ml/min.
Methanizer Installed	Yes or No.
Methanizer Oven	On or Off.
Temperature (°C)	450°C.

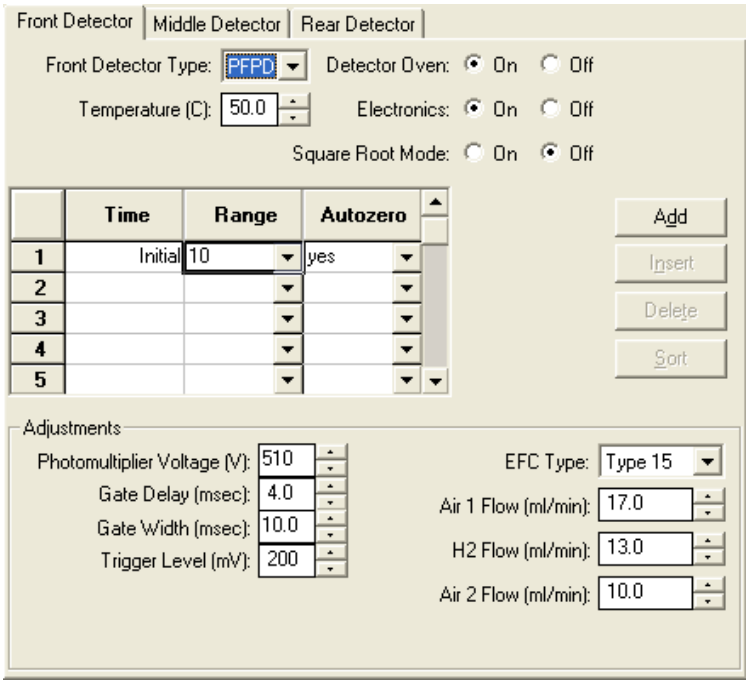
ECD Detector



Item	Description
Detector Oven	On or Off. Turns the TCD oven on or off.
Electronics	On or Off. Indicates whether the installed ECD will be used or not.

Item	Description
Temperature (C)	50- 450 °C.
Time	Initial - 999.99 min.
Range	1 or 10.
Autozero	Yes or No. yes at initial time: the ECD Autozero is on continuous before the run starts. Autozero is automatically disabled once the run starts.
Add	Adds a line to the spreadsheet.
Insert	Inserts a line above the currently selected row in the spreadsheet.
Delete	Deletes the currently selected row(s) in the spreadsheet.
Sort	Sorts the spreadsheet rows by time.
Time Constant	Slow or Fast.
Cell Current	N2 High, N2 Std, CAP, Ar-CH4, Zero.
Contact Potential (mV)	0- 800 mV.
EFC Type	None, Type 13 for the ECD.
Make up Flow (ml/min)	0-50 ml/min.
Methanizer Installed	Yes or No.
Methanizer Oven	On or Off.
Temperature (°C)	450 °C.

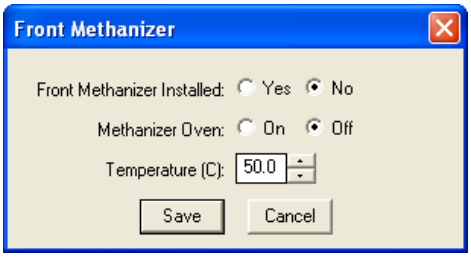
PFPD Detector



Item	Description
Detector Oven	On or Off. Turns the PFPD oven on or off.
Electronics	On or Off. Indicates if the installed PFPD is used.
Temperature (C)	50- 450 °C. Specifies the PFPD Temperature.
Square Root Mode	On or Off.
Time	Initial - 999.99 min.
Range	8, 9, 10.
Autozero	Yes or No Yes at initial time: the PFPD Autozero is on continuous before the run starts. Autozero is automatically disabled once the run starts.
Add	Adds a line to the spreadsheet.
Insert	Inserts a line above the currently selected row in the spreadsheet.
Delete	Deletes the currently selected row(s) in the spreadsheet.
Sort	Sorts the spreadsheet rows by time.
Photomultiplier Voltage (V)	300- 900 V.
Gate Delay (msec)	20 msec.
Gate Width (msec)	20 msec.
Trigger Level (mV)	10- 2000 mV.
EFC Type	None or Type 15 for the PFPD detector.
Air 1 Flow (ml/min)	0- 50 ml/min.
H2 Flow (ml/min)	0- 30 ml/min.
Air 2 Flow (ml/min)	0- 30 ml/min.
Methanizer Installed	Yes or No.
Methanizer Oven	On or Off.
Temperature (°C)	450 °C.

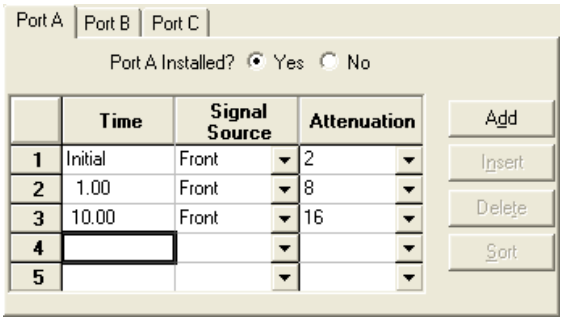
Methanizer Dialog Box

This dialog box is displayed by clicking on the Methanizer button at the bottom of the detector window.



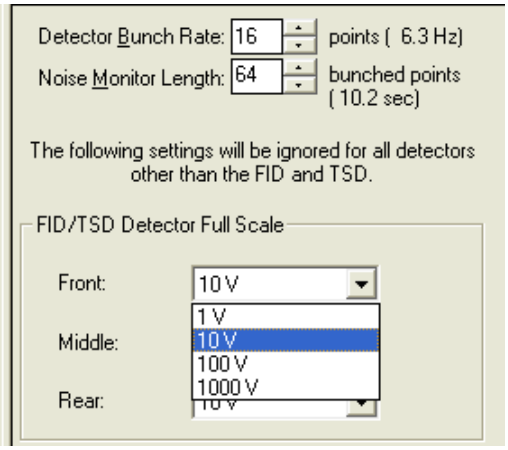
Item	Description
Methanizer Installed	Yes or No.
Methanizer Oven	On or Off.
Temperature (°C)	450 °C.

450-GC Output



Item	Description
Port A Port B Port C	The 450-GC can have up to three output ports installed (A, B, and C). The tabs at the top of the window select the output port position.
Port Installed?	Yes or No. Indicates if the Port at each position is installed. For the installed Port, the Output time program is used to program the detector signal source and attenuation.
Time	Initial - 999.99 min.
Signal Source	Front, Middle, Rear.
Attenuation	Powers of 2 from 1- Infinite.
Add	Adds a line to the spreadsheet.
Insert	Inserts a line above the currently selected row in the spreadsheet.
Delete	Deletes the currently selected row(s) in the spreadsheet.
Sort	Sorts the spreadsheet rows by time.

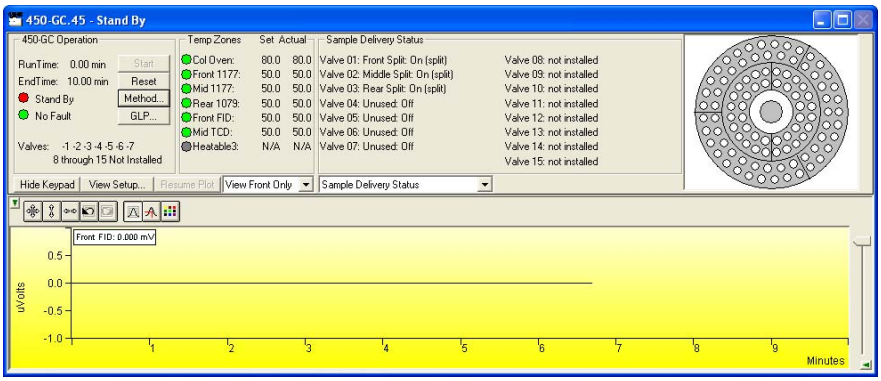
450-GC Data Acquisition



Item	Description
Detector Bunch Rate	Powers of 2 from 1 to 128 points. Sets the detector bunch rate in numbers of points; shows the resulting frequency in Hz. With increased bunch rates, less disk space is required for storing the data. With decreased rates, more data is collected. Bunch rate should be set appropriately for the narrowest peak of interest in your chromatogram.
Monitor Length	16 to 128 bunched points. Sets the number of points collected during the monitoring period, shows the resulting time in seconds. Used to set the number of data points used to calculate the baseline noise. Generally, a larger value entered here will yield a lower noise calculation.
FID/TSD Detector Full Scale (Font, Middle, Rear)	1V, 10V, 100V, 1000V. Specifies the maximum detector value that will be processed by the Varian MS Workstation. The dynamic range of the FID and TSD detectors are equivalent to 1000V full scale, but if your peaks of interest fall significantly below this value, you may wish to limit the full scale value here. *Since the attenuation setting used by the Standard Report application to scale the chromatogram printout is based on the detector's full scale value, a lower full scale value will allow you to scale smaller peaks with greater resolution.*

450-GC System Control Command Reference

Status and Control Window



The 450-GC Status and Control window is divided into five display areas. These are the 450-GC Operation display, the Temp. 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 next display area to the right is the Temp. Zones Status display, which shows the setpoint and current actual temperature of each heated zone in the GC.

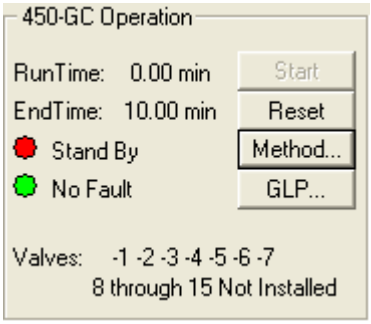
Next is the Component Status display. You select the component for which you wish to see more detailed status information, including ready and fault status for the selected component. You can change the component being displayed using the selection box below the display area, or by clicking on the corresponding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

The Chromatogram is below these display areas. A selection box above the chromatogram allows you to select the channels for which you want to view the realtime chromatogram.

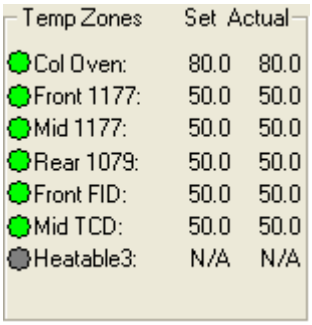
450-GC Operation Display

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



Item	Description
Runtime	Shows the elapsed time in minutes since the beginning of the run. The maximum run time is 999.99 minutes.
Endtime	Shows the time at which the run will end.
State	Ready, Running, Stabilizing, Equilibrating, Computing, Needs Monitor, Monitoring, Sampling, Connecting, or Not Ready Shows 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	Displays 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, 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 450-GC is in the Ready state.
Reset	Resets the GC, advancing it to the next state. If it is 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…	Opens the Method Builder application for editing the active 450-GC method.

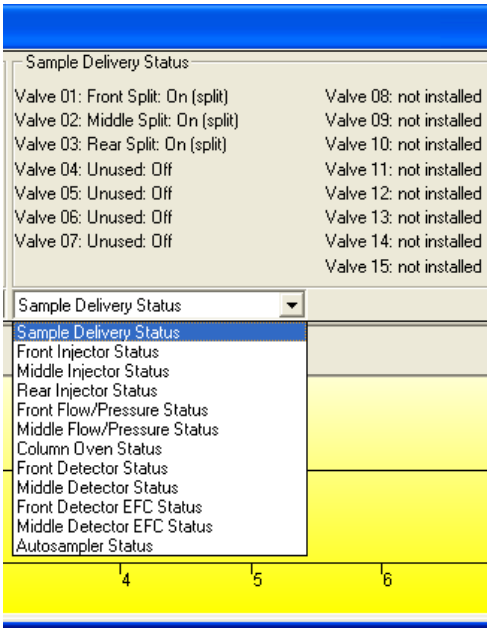
Temp Zones Status Display



The temperature zones status display is in the middle portion of the 450-GC Status and Control window. The display includes the setpoints and actual temperatures of the column oven, the three coolable zones, and the three heatable-only zones of the 450-GC. The display is “Fault” if a fault occurs in the zone component or “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 on one of the temperature zone entries will 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, 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 status to view with the drop down list box below the display area.

Column Oven Status:

Item	Description
Ready	Yes or No. The column oven is Ready (Yes) if the setpoints have been achieved and stabilized. The column oven is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the oven 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. Displays if a fault in the column oven component has occurred.
Oven Power	On or Off. Displays if the column oven component is turned off or on at the 450-GC.
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 at the 450-GC.

Item	Description
Stabilization Time	0.00 to 10.00 min Shows 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 at which the column oven coolant is enabled.
Timeout	0.01 min to 999.99 min Displays the programmed coolant time-out value in the active method for the column oven.
Timed Out	Yes or No. Displays Yes if the coolant time-out period has elapsed for the column oven.

AutoSampler Status:

This option is only displayed 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	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.
Injection Mode	Shows the injection mode specified in the active 450-GC method.
Injection number: x of y	where 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 below.		
	Name	**Default State**	**Energized State**
	Unused	Off	On
	Front Split	On (split)	Off (s/less)
	Middle Split	On (split)	Off (s/less)
	Rear Split	On (split)	Off (s/less)
	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 Det	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	SPT Trap	SPT Desorb
	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. The 1177 injector oven is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the oven becomes not ready or goes “out of tolerance”.
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.

1079 Injector Status:

Item	Description
Ready	Yes or No. The 1079 injector oven is Ready (Yes) if the setpoints have been achieved and stabilized. The 1079 injector oven is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the oven 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. 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.

Item	Description
Split State	On or Off. Displays the current split state of the 1079 injector method.
Split Ratio	1 to 10000 or Off Displays the current split ratio of the 1079 injector method. 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 Displays the programmed injector oven temperature at which the 1079 injector oven coolant is enabled.
Timeout	0.01 min to 999.99 min Displays the programmed coolant time-out value in the active method for the 1079 injector oven.
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. The 1041/1061 injector oven is Ready (Yes) if the setpoints have been achieved and stabilized. The 1041/1061 injector oven is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the oven becomes not ready or goes “out of tolerance”.
Fault	Yes or No. Displays if a fault in the 1041/1061 injector component has occurred.
1041/1061 Oven	On or Off. Displays if the 1041/1061 injector oven component is turned off or on at the 450-GC. The 1041 and 1061 injectors are isothermal injectors.
Setpoint	50 to 450 °C Displays the 1041/1061 injector oven programmed temperature setting in the active method.
Actual	50 to 450 °C Displays the actual temperature of the 1041/1061 injector oven at the 450-GC.

SPT Injector Status:

Item	Description
Ready	Yes or No. The SPT injector oven is Ready (Yes) if the setpoints have been achieved and stabilized. The SPT injector oven is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the oven 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. Displays if a fault in the SPT injector component has occurred.
SPT Oven	On or Off. Displays if the SPT injector oven component is turned off or on at the 450-GC.
Coolant	On or Off. Displays if the SPT injector oven coolant is enabled in the active method.
Setpoint	-99 to 450 °C Displays the SPT injector oven programmed temperature setting in the active method.
Actual	-99 to 450 °C Displays the actual temperature of the SPT injector oven at the 450-GC.
Enable SPT Coolant at	30 °C to 450 °C Displays the programmed injector oven temperature at which the SPT injector oven coolant is enabled.
Timeout	0.01 min to 999.99 min Displays the programmed coolant time-out value in the active method for the SPT injector oven.
Timed Out	Yes or No. Displays Yes if the coolant time-out period has elapsed for the SPT injector oven.

Type 21 or Type 25 Injector EFC Flow/Pressure Status:

Item	Description
Ready	Yes or No. The Type 21 or Type 25 Injector EFC component is Ready (Yes) if the setpoints have been achieved and stabilized. The Type 21 or Type 25 Injector EFC component is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the EFC 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. Displays if a fault in the Type 21 or Type 25 EFC component has occurred.

Item	Description
Type 21 or Type 25 Pressure Setpoint	0.1 to 150 psi Displays the programmed column head pressure setting in the active method.
Actual Pressure	0.1 to 100 psi Displays the actual column head pressure at the 450-GC.
Column Flow	Displays, 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	Displays, 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	Displays, in ml/min, the total flow rate through the system.
Split State	On or Off. Displays the current split state of the 1079/1177 injector method.
Split Ratio	1 to 10000 Displays 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. The Type 23 Injector EFC component is Ready (Yes) if the setpoints have been achieved and stabilized. The Type 23 Injector EFC component is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the EFC 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. Displays if a fault in the Type 23 EFC component has occurred.
Type 23 Flow Setpoint	0.1 to 100 ml/min Displays the programmed column flow rate setting in the active method.
Actual Flow	0.1 to 100 ml/min Displays the actual column flow rate calculated from the measured head pressure and column parameters (carrier gas, column length, and internal diameter).
Pressure	Displays, in psi, the measured column head pressure.
Linear Velocity	Displays, 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. The Type 24 Injector EFC component is Ready (Yes) if the setpoints have been achieved and stabilized. The Type 24 Injector EFC component is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the EFC 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. Displays if a fault in the Type 24 EFC component has occurred.
Type 24 Pressure Setpoint	0.1 to 150 psi Displays the programmed column head pressure setting in the active method.
Actual Pressure	0.1 to 100 psi Displays the actual column head pressure at the 450-GC.
Column Flow	Displays, 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 Displays the programmed total flow rate in the active method.
Linear Velocity	Displays, 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. The TCD detector is Ready (Yes) if the setpoints have been achieved and stabilized. The TCD detector is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the TCD 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. 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 TCD Range initial condition setting or the time-programmed setting in the active method.
Time Const	Fast (50 msec) or Slow (200 msec) Displays the electrometer time constant setting from the TCD Adjustments in the active method.

Item	Description
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 and should normally set around 0%. A large offset in bridge balance (+ or -) could indicate a potential problem.
Polarity	positive or negative Displays the TCD Polarity initial condition setting or time-programmed setting in the active method.
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.

MicroTCD Status:

NOTE: The microTCD detector is set to 110°C and is not adjustable.

Item	Description
Ready	Yes or No. The microTCD detector is Ready (Yes) if the setpoints have been achieved and stabilized. The microTCD detector is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the microTCD 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. Displays if a fault in the microTCD detector component has occurred.
microTCD Electronics	On or Off Displays the microTCD Electronics setting in the active method.
Range	0.05, 0.5, or 5.0 Displays the microTCD Range initial condition setting or the time-programmed setting in the active method.
Time Const	Fast (50 msec) or Slow (200 msec) Displays the electrometer time constant setting from the microTCD Adjustments in the active method.
Current	Displays, in mA, the actual microTCD current.
Balance Pct	Displays, in %, the microTCD bridge balance. On the 450-GC, the bridge is balanced automatically and should normally set around 0%. A large offset in bridge balance (+ or -) could indicate a potential problem.

Item	Description
Polarity	positive or negative Displays the microTCD Polarity initial condition setting or time-programmed setting in the active method.
Detector Signal	Displays, in mV, the actual microTCD 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) if the setpoints have been 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. Displays if a fault in the FID detector component has occurred.
FID Electronics	On or Off Displays the FID Electronics setting in the active method.
Range	9, 10, 11, or 12 Displays the FID Range initial condition setting or the time-programmed setting in the active method.
Time Const	Fast (50 msec) or Slow (200 msec) Displays the electrometer time constant setting from the FID Adjustments in the active method.
Detector Signal	Displays, in mV, the actual FID detector signal at the 450-GC.
Bunch Size	Displays the data acquisition bunch size.
Freq	Displays the data acquisition bunch rate, in Hz.

ECD Status:

Item	Description
Ready	Yes or No. The ECD detector is Ready (Yes) if the setpoints have been achieved and stabilized. The ECD detector is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the ECD 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.

Item	Description
	Displays if a fault in the ECD detector component has occurred.
ECD Electronics	On or Off Displays the ECD Electronics setting in the active method.
Range	1 or 10 Displays the ECD Range initial condition setting or the time-programmed setting in the active method.
Time Const	Fast (50 msec) or Slow (200 msec) Displays the electrometer time constant setting from the ECD Adjustments in the active method.
Detector Signal	Displays, in mV, the actual ECD detector signal at the 450-GC.
Bunch Size	Displays the data acquisition bunch size.
Freq	Displays the data acquisition bunch rate, in Hz.

TSD Status:

Item	Description
Ready	Yes or No. The TSD detector is Ready (Yes) if the setpoints have been achieved and stabilized. The TSD detector is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the TSD 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. Displays if a fault in the TSD detector component has occurred.
TSD Bead Power	On or Off Displays the TSD Bead Power initial condition setting or the time-programmed setting in the active method.
Range	9, 10, 11, or 12 Displays the TSD Range initial condition setting or the time-programmed setting in the active method.
Time Const	Fast (50 msec) or Slow (200 msec) Displays the electrometer time constant setting from the TSD Adjustments in the active method.
Bead Current	2.4 to 3.8 A or Off Displays the TSD Bead Current setting in the active method or Off if the Bead Power is off.
Detector Signal	Displays, in mV, the actual TSD detector signal at the 450-GC.
Bunch Size	Displays the data acquisition bunch size.
Freq	Displays the data acquisition bunch rate, in Hz.

PFPD Status:

Item	Description
Ready	Yes or No. The PFPD detector is Ready (Yes) if the setpoints have been achieved and stabilized. The PFPD detector is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the PFPD 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. Displays if a fault in the PFPD detector component has occurred.
PFPD Electronics	On or Off Displays the PFPD Electronics setting in the active method.
Range	8, 9, or 10 Displays the PFPD Range initial condition setting or the time-programmed setting in the active method.

Type 11 Detector EFC Status:

Item	Description
Type	11 Displays the Detector EFC type. Detector EFC Type 11 has 3 channels and is used for FID detector gas control.
Ready	Yes or No. The Detector EFC is Ready (Yes) if the setpoints have been achieved and stabilized. The Detector EFC is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the Detector EFC 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. Displays if a fault in the Detector EFC component has occurred
Ch 1 (Make up) Set, Actual	Displays, in ml/min, the programmed and actual channel 1 flow rate.
Ch 2 (H2) Set, Actual	Displays, in ml/min, the programmed and actual channel 2 flow rate.
Ch 3 (Air) Set, Actual	Displays, in ml/min, the programmed and actual channel 3 flow rate.

Type 12 Detector EFC Status:

Item	Description
Type	12 Displays the Detector EFC type. Detector EFC Type 12 has 3 channels and is used for TSD detector gas control.
Ready	Yes or No.
Fault	Yes or No.
Ch 1 (Makeup) Set, Actual	Displays, in ml/min, the programmed and actual channel 1 flow rate.
Ch 2 (H2) Set, Actual	Displays, in ml/min, the programmed and actual channel 2 flow rate.
Ch 2 (Air) Set, Actual	Displays, in ml/min, the programmed and actual channel 3 flow rate.

Type 13 Detector EFC Status:

Item	Description
Type	13 Displays the Detector EFC type. Detector EFC Type 13 has 1 channel and is used for either ECD or TCD detector gas control.
Ready	Yes or No.
Fault	Yes or No.
Ch 1 (Makeup) Set, Actual	Displays, in ml/min, the programmed and actual channel 1 flow rate for TCD detector gas control.
Ch 1 (Reference) Set, Actual	Displays, in ml/min, the programmed and actual channel 1 flow rate for ECD detector gas control.

Type 14 Detector EFC Status:

Item	Description
Type	14 Displays the Detector EFC type. Detector EFC Type 14 has 2 channels and is used for TCD detector gas control.
Ready	Yes or No.
Fault	Yes or No.
Ch 1 (Make up) Set, Actual	Displays, in ml/min, the programmed and actual channel 1 flow rate.
Ch 2 (Reference) Set, Actual	Displays, in ml/min, the programmed and actual channel 2 flow rate if the channel 2 gas type is a Helium, Nitrogen, or Argon reference.
Ch 2 (Make up) Set, Actual	Displays, in ml/min, the programmed and actual channel 2 flow rate if the channel 2 gas type is a Helium, Nitrogen, or Argon make-up.

Type 15 Detector EFC Status:

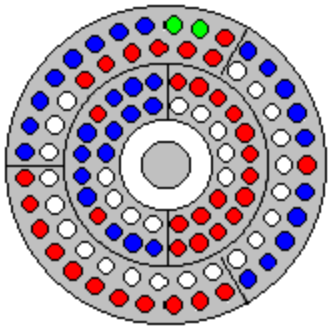
Item	Description
Type	15 Displays the Detector EFC type. Detector EFC Type 15 has 3 channels and is used for PFPD detector gas control.
Ready	Yes or No.
Fault	Yes or No.
Ch 1 (Air 1) Set, Actual	Displays, in ml/min, the programmed and actual channel 2 flow rate.
Ch 2 (H2) Set, Actual	Displays, in ml/min, the programmed and actual channel 2 flow rate.
Ch 3 (Air 2) Set, Actual	Displays, in ml/min, the programmed and actual channel 2 flow rate.

Type 16 Detector EFC Status:

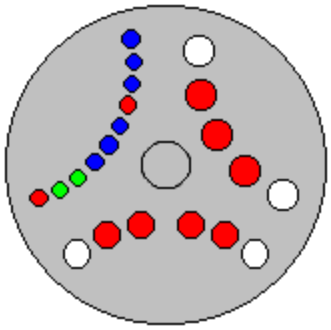
Item	Description
Type	16 Displays the Detector EFC type. Detector EFC Type 16 has 2 channels and is used for TCD detector gas control.
Ready	Yes or No.
Fault	Yes or No.
Ch 1 (Make up) Set, Actual	Displays, in ml/min, the programmed and actual channel 1 flow rate.
Ch 2 (Reference) Set, Actual	Displays, in ml/min, the programmed and actual channel 2 flow rate if the channel 2 gas type is a Hydrogen reference.
Ch 3 (Make up) Set, Actual	Displays, in ml/min, the programmed and actual channel 2 flow rate if the channel 2 gas type is a Hydrogen make-up.

8400/8410 Carousel Display

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



8400 AutoSampler Carousel



8410 AutoInjector Carousel

Item	Description
Red fill	Indicates vials listed in the active SampleList that have not yet been sampled or are missing.
Green fill	Indicates the vial (vials in Dual Mode) currently being sampled.
Blue fill	Indicates the vials in the active SampleList that have been sampled.

Action	Description
Click a vial position	Displays the vial number for that position for 5 seconds
Double-click a vial position	Opens the Inject Single Sample dialog box to inject a single sample.

Chromatogram Display Toolbar

	Shows or hides the toolbar.
	Full Scale: zooms all traces to their full scale values. This button is the same as double clicking in the chromatogram display window.
	Vertical Full Scale: the chromatogram is zoomed such that all of the trace is visible within the given time range. This command only affects the displayed amplitude range, the time range is unaffected. This button is the same as double clicking in the Y axis of the chromatogram display window.
	Horizontal Full Scale: the chromatogram is zoomed such that the entire time range is visible. This command only affects the displayed time range, the amplitude range is unaffected. This button is the same as double clicking in the X axis of the chromatogram display window.
	Previous Scaling: zooms to the previous time and amplitude range. Each time you scale the chromatogram, the new scaling rectangle is added to the end of a list of scaling rectangles. Previous scaling zooms the display to the value stored in the previous position on the list. This item is disabled when at the start of the list.
	Next Scaling: zooms to the next time and amplitude range. Each time you scale the chromatogram, the new scaling rectangle is added to the end of a list of scaling rectangles. Next scaling zooms the display to the value stored in the next position on the list. Since new scaling rectangles are added to the end of the list, it implies that Next Scaling is only available when you had formerly hit the Previous Scaling button. That is, this item is disabled when at the end of the list.
	Autoscaling: when depressed, the vertical axis is autoscaled continuously. If the chromatogram trace exceeds the current vertical scaling, the Y axis is automatically adjusted to keep the trace in view.
	Cursor Display: turns the cursor on or off. The cursor follows the chromatogram trace and displays the time and amplitude of its current position in an “info-panel. Hold the control key down to allow the cursor to move anywhere on the screen without following the active trace.

Chromatogram Zooming and Scrolling

The following mouse actions are possible for the chromatogram display window:

Action	Effect of Action
Left mouse button click and drag a selection.	Expands selected section of chromatogram to fill the entire window.
Left mouse button double click.	Zooms to full scale.
Left mouse click and hold	Zooms isometrically from the mouse position, or, if you are holding the control key down, zooms out from that point. Once PowerZooming begins, you can move the mouse around while the mouse button is still down to change the point at which you are zooming

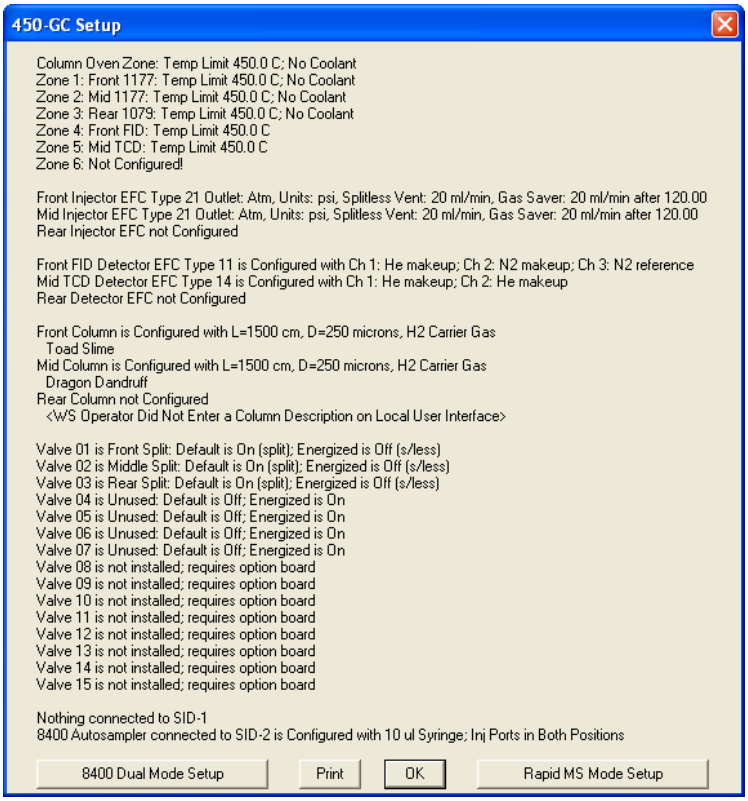
You can view other sections of the chromatogram while maintaining the same zoom level by scrolling. Scroll bars are displayed only if the time or amplitude range of your zoomed view is less than the maximum time or amplitude range of the chromatogram. Scrolling horizontally lets you see sections of the chromatogram earlier or later than the current section. Scrolling vertically lets you see sections of higher or lower amplitude.

You can scale vertically using the Attenuation Control to the right of the chromatogram display window. This adjusts the amplitude range on a logarithmic scale. When using the attenuation control, the lowest point of the active trace is fixed, and the amplitude range is adjusted to a smaller range as you slide the position indicator up and to a larger range as you slide it down.

You can zoom in the amplitude and time axes in the same way as you do in the chromatogram display window. You can select a rectangular section of the axis, PowerZoom, and double click in the axis. These actions zoom just like they would in the chromatogram display window, except that only the amplitude scaling is affected when zooming in the amplitude axis and only the time scaling is affected when zooming in the time axis.

450-GC Setup Dialog Box

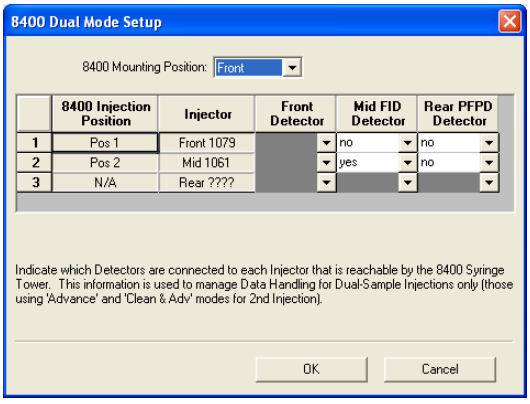
This dialog box shows the hardware configuration reported by the 450-GC. This configuration is compared to and must match the configuration in the Method when it is activated.



8400/8410 Dual Mode Setup Dialog Box

When the 8400 AutoSampler or 8410 AutoInjector is used in Dual Mode, this dialog box is used 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 injected sample and the other for the second injected sample.

The samples are identified by their 8400/8410 Injection Position, for example, Position 1 or Position 2. The table in this dialog box allows the user to specify which detector information to associate with each 8400/8410 Injection Position.

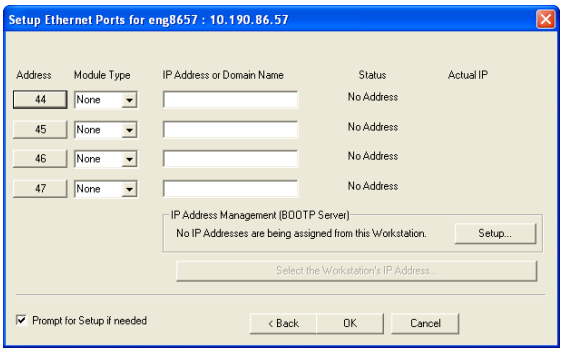


After the correct 8400/8410 Mounting Position, Front or Rear, is entered, the Injector that corresponds to each 8400/8410 Injection Position is identified. The 8400/8410 Mounting Position specified in this dialog box has no effect on the actual operation of the AutoSampler. It is for informational purposes only.

Field	Description
8400/8410 Mounting Position (Informational entry only)	Front or Rear When set to match the physical mounting location of the 8400/8410, the Injector column in the table will show the 450-GC injector that corresponds to the 8400/8410 Injection Positions. The 8400/8410 Mounting Position specified in this Dialog box has no effect on the actual operation of the 8400/8410 AutoSampler.
8400/8410 Injection Position (not user modifiable)	Pos 1 and Pos 2 Specifies the 8400/8410 Injection Position for the other entries in the row.
Injector (not user modifiable)	When the 8400/8410 Mounting Position is set to match the physical mounting location of the 8400/8410, this column will show the 450-GC injector that corresponds to each of the 8400/8410 Injection Positions. This column is for informational use only and does not affect the operation of the 8400/8410 AutoSampler or Workstation.
Front XXXX Detector where XXXX is the abbreviation for the type of detector	Yes or No When yes is selected, the chromatographic data from this detector channel will be added to the datafile created for the sample injected in the 8400/8410 Injection Position specified on the same line in the first column of the row.
Mid XXXX Detector where XXXX is the abbreviation for the type of detector	Yes or No When yes is selected, the chromatographic data from this detector channel will be added to the datafile created for the sample injected in the 8400/8410 Injection Position specified on the same line in the first column of the row.
Rear XXXX Detector where XXXX is the abbreviation for the type of detector	Yes or No When yes is selected, the chromatographic data from this detector channel will be added to the datafile created for the sample injected in the 8400/8410 Injection Position specified on the same line in the first column of the row.

Setup Ethernet Ports Dialog Box

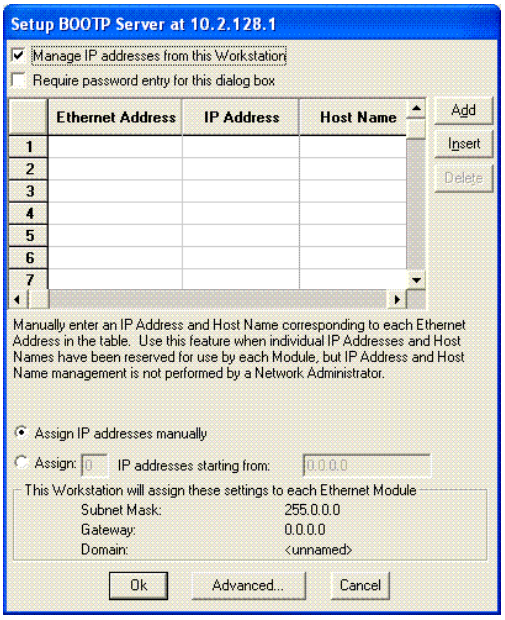
This is displayed the first time that Workstation guides you through the setup of your 450-GC in System Control. This dialog box is also accessed from the Instrument/Setup Ethernet Communications menu item of System Control.



Field	Description	
Address	44, 45, 46, or 47 Click the Address button to attach to a 450-GC on the Ethernet network. If you are running on a company network, only GCs on the same local subnet appear in the Select Available Modules dialog box that is displayed after clicking the Address button.	
Module Type	None or 450-GC This field is set if you select a 450-GC using the Address button. If you specify an IP Address or Domain Name explicitly, then select 450-GC from this combobox.	
IP Address or Domain Name	This field is set if you select a 450-GC using the Address button. To connect to a GC in a different subnet, type its IP Address directly into the IP Address or Domain Name field.	
Status	Available, Online, In Use By <client>, Not Responding, or No Address Displays the connection status of the 450-GC.	
	Status	Meaning
	Available Online In Use By <client> Not Responding No Address	Not in use by anyone In use by this Workstation In use by another Workstation Not responding to Workstation queries No IP Address or name specified
Actual IP	Displays the actual IP address of the connected 450-GC.	
Setup...	Click to setup IP address management (BOOTP Server). The Setup BOOTP Server Dialog Box is displayed.	
Select the Workstation IP Address...	Allows you to select from one of the IP addresses configured for this computer.	

Setup BOOTP Server Dialog Box

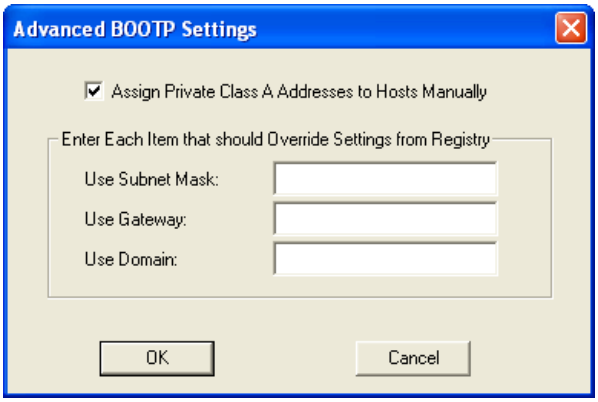
If IP addresses are managed by a Network Administrator from a central source, the 450-GCs must be added to the list of devices requiring IP addresses. IP addresses must be assigned to GCs using a BOOTP Server. A BOOTP Server lists Ethernet addresses (which are unique to each communication card installed in each 450-GC) along with the IP addresses that are to be assigned to the corresponding device. You may obtain the Ethernet address for each 450-GC from the GC's front panel. Turn on the 450-GC and press any key to allow it to start in local mode.



Field	Description
Manage IP addresses from this Workstation	Checked or not checked. When IP addresses are managed from a central location by a Network Administrator, the BOOTP Server on your Workstation must be disabled (not checked).
Require password entry for this dialog box	Checked or not checked. Check this box to restrict access to the BOOTP Server dialog box to avoid inadvertent or unauthorized changes to IP address assignments. If this item is checked, the next time you enter the BOOTP Server dialog box, you will be prompted for a password. The initial password is blank (no password). To set your password initially, enter the desired password in the Enter new password and Re-enter new password fields. Subsequent entry into the BOOTP Server will require this password.
Ethernet Address	Displays the Ethernet address of any 450-GCs already connected to the network and powered on. You may also manually enter an Ethernet address for a 450-GC (available from the 450-GC front panel display).
IP Address	Displays the IP address of any 450-GCs already connected to the network and powered on. You may also manually enter an IP address for a 450-GC. Use

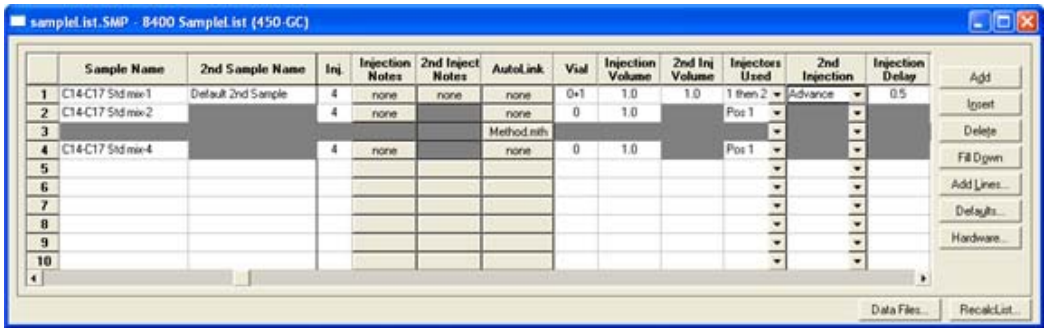
Field	Description
	the manual entry of IP addresses and Host Names when individual IP addresses have been reserved for use by each 450-GC but IP Address and Host Name management is not performed by a Network Administrator.
Host Name	You must enter a name for each 450-GC. The IP address will not be assigned to the GC until a name is entered.
Assign IP addresses manually	Selected or not selected Select this entry if you manually enter IP addresses and Host Name entries in the table.
Assign IP addresses starting from	Selected or not selected Select this entry to consecutively assign IP addresses beginning from a particular address. Enter the number of IP addresses to assign automatically and the starting IP address. As 450-GCs are powered on, IP addresses are automatically assigned from the specified address.
Subnet Mask	Displays the subnet mask assigned to the Workstation. This parameter is assigned in the TCP/IP network setup in the Control Panel application.
Gateway	Displays the Gateway assigned to the Workstation. This parameter is assigned in the TCP/IP network setup in the Control Panel application.
Domain	Displays the Domain name assigned to the Workstation. This parameter is assigned in the TCP/IP network setup in the Control Panel application.
Advanced…	Click for specialized IP address management entries. The Advanced BOOTP Dialog Box is displayed.

Advanced BOOTP Settings Dialog Box



Item	Description
Assign Private Class A addresses to Hosts Manually	Checked or not checked Determines whether IP addresses must be entered in the Setup BOOTP Server dialog box (checked) or if they are generated (unchecked).
Use Subnet Mask	Enter the subnet mask here. This is only used when the Manage IP addresses from this Workstation checkbox is checked in the Setup BOOTP Server dialog box.
Use Gateway	Enter the gateway address here. This is only used when the Manage IP addresses from this Workstation checkbox is checked in the Setup BOOTP Server dialog box.
Use Domain	Enter the domain name here. This is only used when the Manage IP addresses from this Workstation checkbox is checked in the Setup BOOTP Server dialog box.

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 displayed and available for editing when the 8400 AutoSampler or 8410 AutoInjector is used in Duplicate Mode or

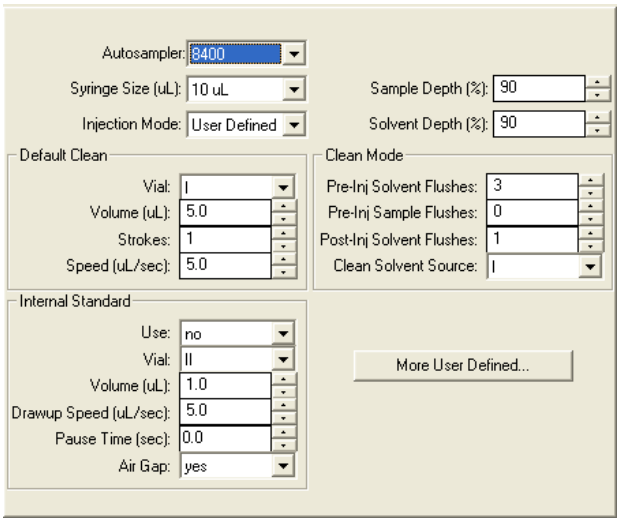
Dual Mode. Refer to the help on the generic SampleList Window for a description of the fields not listed below.

Field	Description
2nd Sample Name (Dual Mode operation only)	Up to 19 characters Sets the name of the second sample injected. This column is only displayed when the 2nd Injection is "Advance" or "Clean & Adv".
2nd Inject Notes (Dual Mode operation only)	up to 180 characters Opens the Notes window for the selected second sample to edit or create a note about the sample. This column is only displayed when the 2nd Injection is "Advance" or "Clean & Adv".
Vial	0 through 99 for 8400 AutoSampler 1 through 21 for 8410 AutoInjector Sets the AutoSampler vial number of each sample in the SampleList. When the 2nd Injection is "Advance" or "Clean & Adv", two sequentially numbered vials will be displayed. The first vial will be injected on the first injection and the next vial location will be sampled for the second injection.
Injection Volume	0.1 to 10 µL Sets 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 exceed the syringe volume, a 450-GC hardware fault will occur. This will cause 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 displayed 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 10 µL Sets 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 will occur. This will cause 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 displayed in the 450-GC setup screen, you should begin the SampleList at the selected line to

Field	Description
	bypass the samples that have already been run.
Injectors Used	Pos 1, Pos 2, 1 then 2, or 2 then 1 Selects the 8400 Injection position to be used for the sample. If the 8400 is not configured for both injection positions, entering the wrong position will cause the sample line to be skipped and a “Bad Injector” message entered into the message log. To run samples in Duplicate Mode or Dual Mode, you must 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 will take before making the second injection during a run. If you choose “Duplicate” or “Clean & Dup”, the same sample will be used for both injections. This is called Duplicate Mode. If you choose “Advance” or “Clean & Adv”, the 8400 will advance to the next vial location and will sample the vial, if any, that is there for the second sample injection. This is called Dual Mode.
Injection Delay (Duplicate Mode or Dual Mode operation only)	0.0 and 0.1 through 10.0 minutes Sets 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 will prepare and load the syringe for the second injection. When the syringe is loaded, it will move to the inject position and wait 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 placed in the message log.

431-GC Method Command Reference

431-GC AutoSampler

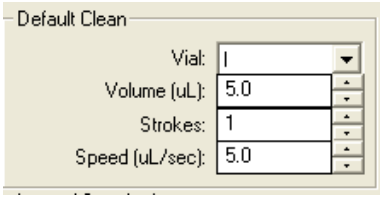


When the 8400 AutoSampler or 8410 AutoInjector is selected, the AutoSampler window may contain up to five sections. The topmost section is common to all modes of operation. The entries in this section are described below.

In addition, all modes of operation also include a Default Clean section and a Clean Mode section. When Viscous, Volatile, or User Defined modes are selected, the Internal Standard section is displayed. In User Defined mode, the “More User Defined…” button is displayed to provide access to the dialog box to set the User Defined parameters. The Default Settings for Predefined AutoSampler Modes contains a table showing the parameters that are used by the 8400/8410 for each of the predefined modes of operation.

Item	Description
AutoSampler Type	8400, 8410, or None Specifies whether or not an 8400 AutoSampler or 8410 AutoInjector is installed on the 431-GC. If an 8400 or 8410 is not installed on the GC or is turned off, select None. When 8400 or 8410 is selected, the following items are displayed for editing.
Syringe Size (uL)	5 uL or 10 uL Selects the size of the syringe that is installed on the 8400/8410 for use with this method. A 5 microliter or a 10 microliter syringe may be used with the 8400/8410.
Injection Mode	Std Split/Splitless, Std On Column, Neat, Viscous, Volatile, or User Defined Sets the 8400/8410 parameters for the predefined modes of operation.
Sample Depth (%)	0 to 100 % Specifies how far the syringe needle is to go down into the sample vial. 100% is the bottom of the vial. 0% is the bottom of the vial septum.
Solvent Depth (%)	0 to 100 % Specifies how far the syringe needle is to go down into the solvent vial. 100% is the bottom of the vial. 0% is the bottom of the vial septum.

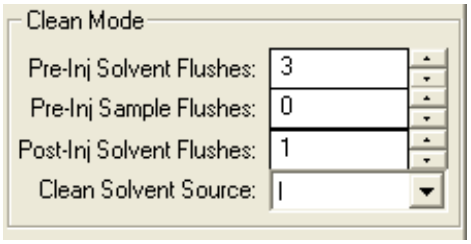
Default Clean Section



Default Cleaning occurs when the Stop button on the front panel of the 431-GC, the Reset button on the 431-GC Status Window in Workstation System Control, or the Stop Automation menu item in Workstation System Control Automation menu is pressed after the 8400/8410 has started its run and before it has finished its sampling and post-injection washing operations. Default Cleaning also occurs when the 431-GC has a fatal automation fault after the 8400/8410 has started its run and before it has finished its sampling and post-injection washing operations.

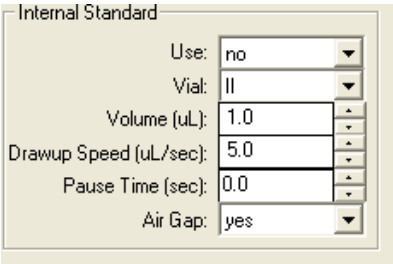
Item	Description
Vial	I, II, or III Specifies which of the three solvent vials will be used by the Default Cleaning
Volume (uL)	0 to 10.0 microliters with 10 uL syringe 0 to 5.0 microliters with 5 uL syringe Specifies the amount of cleaning solvent that will be drawn up with each syringe cleaning stroke.
Strokes	0 to 10 Specifies the number of times the cleaning solvent will be drawn up into the syringe and expelled into the waste cup.
Speed (uL/sec)	0.1 to 50.0 microliters per second with 10 uL syringe 0.1 to 25.0 microliters per second with 5 uL syringe Specifies the speed at which the cleaning solvent will be drawn up into the syringe and the speed at which it is expelled into the waste cup.

Clean Mode Section



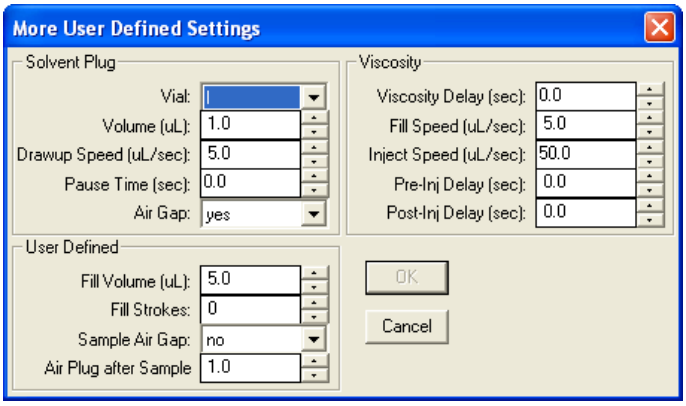
Item	Description
Pre-Inj Solvent Flushes	0 to 99 Specifies the number of times each selected cleaning solvent will be drawn up into the syringe and expelled into the waste cup before flushing with next cleaning solvent (if more than one cleaning solvent source is specified) or the sample.
Pre-Inj Sample Flushes	0 to 99 Specifies the number of times the sample will be drawn up into the syringe and expelled into the waste cup before the syringe is loaded for injection.
Post-Inj Solvent Flushes	0 to 99 Specifies the number of times each selected cleaning solvent will be drawn up into the syringe and expelled into the waste cup before flushing with next cleaning solvent (if more than one cleaning solvent source is specified).
Clean Solvent Source	I, II, III, I & II, I & III, II & III, or I & II & III Selects which solvent vial or sequence of solvent vials will be used to flush the syringe before and after injection.

Internal Standard Section



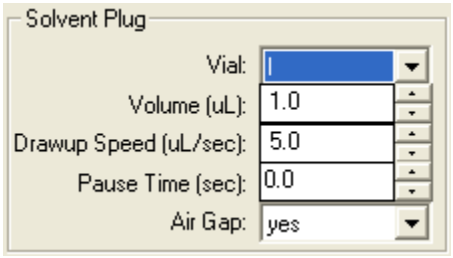
Item	Description
Use	Yes or No If Yes, an internal standard addition will be used. When internal standard addition is used, the internal standard solution will be drawn up into the syringe from the specified solvent vial before the sample is drawn up.
Vial	I, II, or III Selects which solvent vial contains the internal standard.
Volume (uL)	0 to 9.0 microliters with 10 uL syringe 0 to 4.9 microliters with 5 uL syringe Specifies the amount of internal standard to be drawn into the syringe before the sample.
Drawup Speed (uL/sec)	0.1 to 50.0 microliters per second with 10 uL syringe 0.1 to 25.0 microliters per second with 5 uL syringe Specifies the speed at which the internal standard will be drawn up into the syringe.
Pause Time (sec)	0 to 9.9 seconds Specifies how long the syringe is to remain in the internal standard vial after drawing up the internal standard.
Air Gap	Yes or No If Yes, 1 microliter of room air will be drawn into the syringe to create an air gap between the internal standard and the sample.

More User Defined Settings Dialog Box



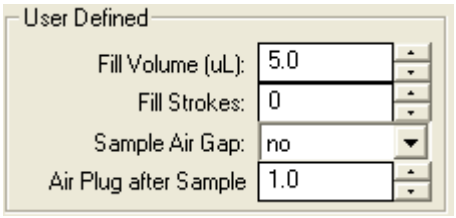
This dialog box is accessed from “More User Defined…” button that is displayed when the User Defined mode is selected.

Solvent Plug Settings



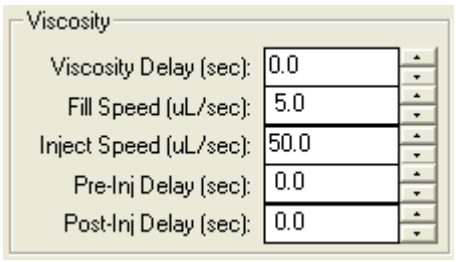
Item	Description
Vial	I, II, or III Selects which solvent vial to use for the solvent plug.
Volume (uL)	0 to 10.0 microliters with 10 uL syringe 0 to 5.0 microliters with 5 uL syringe Specifies the amount of solvent to be drawn into the syringe before the sample or internal standard.
Drawup Speed (uL/sec)	0.1 to 50.0 microliters per second with 10 uL syringe 0.1 to 25.0 microliters per second with 5 uL syringe Specifies the speed at which the solvent will be drawn up into the syringe.
Pause Time (sec)	0 to 9.9 seconds Specifies how long the syringe is to remain in the solvent vial after drawing up the solvent.
Air Gap	Yes or No If Yes, 1 microliter of room air will be drawn into the syringe to create an air gap before the solvent plug.

User Defined Settings



Item	Description
Fill Volume (uL)	0 to 10.0 microliters with 10 uL syringe 0 to 5.0 microliters with 5 uL syringe Specifies the sample volume that will be used for each fill stroke.
Fill Strokes	0 to 99 Specifies the number of the times the sample will be "pumped" in and out of the syringe before loading the sample volume into the syringe.
Sample Air Gap	Yes or No If Yes, 1 microliter of room air will be drawn into the syringe to create an air gap before the sample plug.
Air Plug after Sample	0 to 10.0 microliters with 10 uL syringe 0 to 5.0 microliters with 5 uL syringe Specifies the volume of room air that will be drawn into the syringe after it is loaded with sample.

Viscosity Settings



Item	Description
Viscosity Delay (sec)	0 to 9.9 seconds Specifies how long the syringe is to remain in the sample vial after drawing up the sample.
Fill Speed (uL/sec)	0.1 to 50.0 microliters per second with 10 uL syringe 0.1 to 25.0 microliters per second with 5 uL syringe Specifies the speed at which the sample will be drawn up into the syringe.
Inject Speed (uL/sec)	0.1 to 50.0 microliters per second with 10 uL syringe 0.1 to 25.0 microliters per second with 5 uL syringe Specifies the speed at which the contents of the syringe will be expelled into the injector.

Item	Description
Pre-Inj Delay (sec)	0 to 99.9 seconds Specifies the length of time the syringe needle resides in the injector before expelling the syringe contents.
Post-Inj Delay (sec)	0 to 99.9 seconds Specifies the length of time the syringe needle remains in the injector after expelling the syringe contents.

Default Settings for Predefined AutoSampler Modes

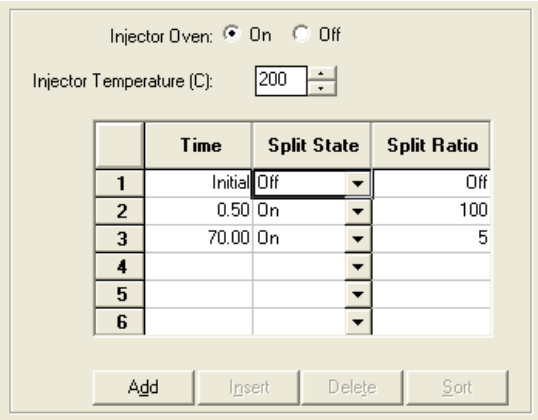
The following table lists the parameter settings used for each of the Predefined 8400/8410 modes using a 10 microliter syringe. If the predefined modes do not work acceptably for your samples, use the User Defined mode to enter settings that will work better with your samples. The values listed in this table provide a starting point for setting the various parameters.

Parameter	Std Split/ Splitless	Std On-Column	Neat	Volatile	Viscous
Solvent Plug Settings:	Solvent plug is not used with predefined modes. If you wish to use solvent plug injections, you must use User Defined mode.				
PreDefined Settings:					
Fill Volume	7.5 uL	7.5 uL	Not used	Not used	Not used
Fill Strokes	5	5	0 ⊕	0	0
Sample Air Gap	No	No	No	No	No
Air Plug after Sample	1 uL	1 uL	1 uL	1 uL	1 uL
Viscosity Settings:					
Viscosity Delay	0 sec	0 sec	0 sec	6 sec	9.9 sec
Fill Speed	2 uL/sec	2 uL/sec	2 uL/sec	1 uL/sec	1 uL/sec
Inject Speed	50 uL/sec	2 uL/sec	50 uL/sec	1 uL/sec	5 uL/sec
Pre-Inj Delay	0 sec	0 sec	0 sec	0 sec	0 sec
Post-Inj Delay	0 sec	6 sec	0 sec	0 sec	12 sec

⊕ Instead of fill strokes Neat mode fills the syringe with sample at 2 uL/sec then expels it into the waste cup at 50 uL/sec. It does this a total of six times. Then it fills the syringe with sample at 2 uL/sec and expels it back into the sample vial at 50 uL/sec. This “pumping” action is done three times. After this is completed, the sample is loaded into the syringe and injected using the parameters in the table.

431-GC Injector Section

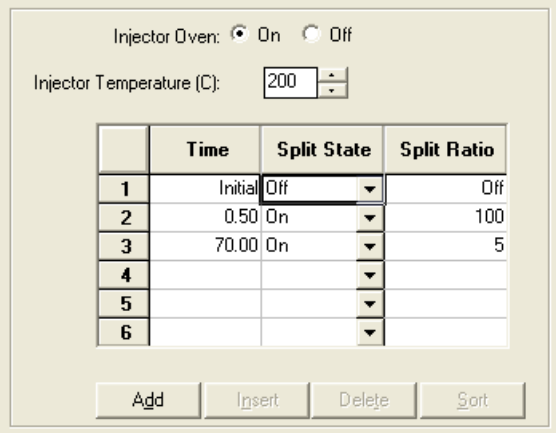
1177 Injector



Item	Description
Injector Oven	On or off. Turns the 1177 injector oven in the selected position on or off.
Temperature (C)	50 to 450C. Specifies the oven temperature.

Spilt Ratio Dialog Box

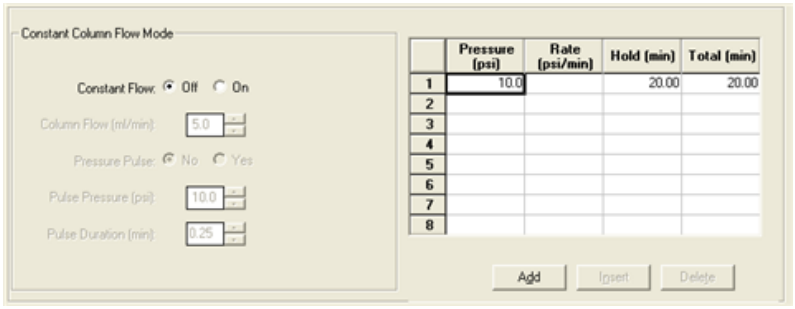
This dialog is displayed from the 431-GC Injector section when an 1177 Injector is configured with Type 21 EFC.



Item	Description
Time	0.00 to 999.99 min.
Split State	On/Off. If the split state is ON, then the sample is split according to the split ratio specified. If the split state is OFF, then all the sample enters the column.
Split Ratio	Off, 1 to 10,000. Use a split ratio of 100 after injection to vent the injector. Use a very low split ratio after flushing to conserve carrier gas.
Add	Adds a line to the spreadsheet.
Insert	Inserts a line above the currently selected row in the spreadsheet.
Delete	Deletes the currently selected row(s) in the spreadsheet.
Sort	Sorts the spreadsheet rows by time.

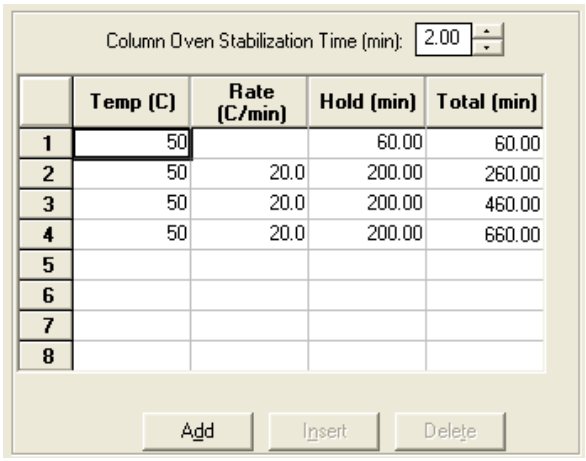
431-GC Flow/Pressure Section

Type 21 (for 1177 injector)



Item	Description
Pressure (psi)	0.1 to 100.0 psi.
Rate (psi/min)	0.01 to 400.00 psi/min. The Rate in the first row is always blank and cannot be edited.
Hold (min)	0.01 to 999.99 min.
Total (min)	0.01 to 999.99 min. Cannot be edited.
Constant Flow	On or Off Click on Constant flow to disable the spreadsheet and reveals the constant flow rate value.
Column Flow (ml/min)	Specifies the desired constant Column Flow.
Pressure Pulse	Yes or No Click on Yes to enable a pressure pulse injection in constant flow mode.
Pressure Pulse (psi)	0.1 to 100.0 psi. Specifies the desired column head pressure during injection.
Pulse Duration (min)	0.01 to 5.00 min. Specifies the period of time after the run starts for which the pressure will be maintained.
Add	Adds a line to the spreadsheet.
Insert	Inserts a line above the currently selected row in the spreadsheet.
Delete	Deletes the currently selected row(s) in the spreadsheet.

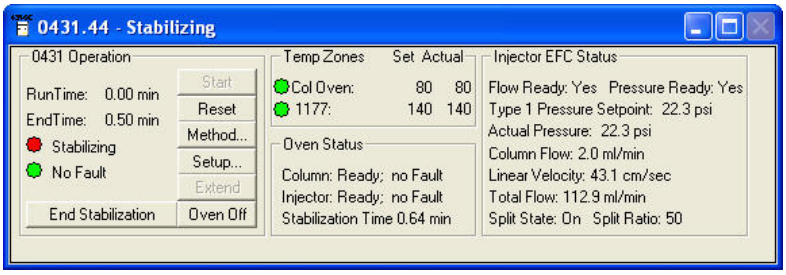
431-GC Column Oven Section



Item	Description
Stabilization Time (min)	10.0 min. Specifies the column Stabilization Time.
Temp (C)	30 - 450 C.
Rate (C/min)	0.01- 100.0 C/min. The Rate in the first row is always blank and cannot be edited.
Hold (min)	0.01-999.99 min.
Total (min)	0.01-999.99 min. Cannot be edited. Column Oven End Time (Total) is displayed in all time-programmed windows of the Method.
Add	Adds a line to the spreadsheet.
Insert	Inserts a line above the currently selected row in the spreadsheet.
Delete	Deletes the currently selected row(s) in the spreadsheet.

431-GC System Control Command Reference

Status and Control Window



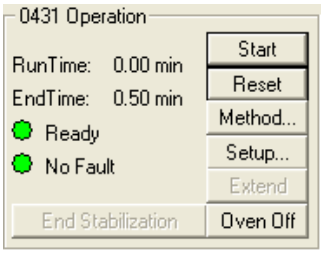
The 431-GC Status and Control window is divided into four display areas. The left-most display area is the 431-GC Operation Display, which contains information about the current run and the overall state of the GC.

The middle displays area is the temperature zone status display, showing the setpoint and current actual temperature of each heated zone in the GC, the Oven Status, and the Injector EFC Status display.

The right most display is the 8400/8410 carousel display.

431-GC Operation Display

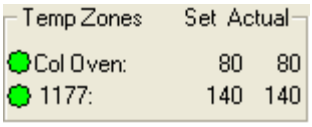
The 431-GC operation display is in the left portion of the 431-GC Status and Control window.



Item	Description
Runtime	Shows the elapsed time in minutes since the beginning of the run. The maximum run time is 999.99 minutes.
Endtime	Shows the time at which the run will end.

Item	Description
State	Ready, Running, Stabilizing, Equilibrating, Computing, or Not Ready Shows 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.
Start	If the system is Ready, starts the GC Method and sends a start signal to the GC. The Start button is disabled unless the 431-GC is in the Ready state.
Reset	Resets the GC, advancing it to the next state. If it is RUNNING, the GC aborts the current run, goes to the READY state, and continues with the next injection in the Sequence.
Method	Opens the Method Builder application for editing the active 431-GC method.
Setup	Opens the GC Setup Dialog Box which is used to set the configuration of the 431-GC.
Extend	The Extend runtime button allows the runtime to be extended by 10 minutes each time the button is clicked on. The extended run time will be used until the method is either re-activated or a new method is activated. The extend run feature does not change the method stored in your MS Workstation.
Oven Off/Oven On	Oven On/Oven Off. Turn the column oven heater either on or off depending on its current state.
End stabilization	If the 431-GC is in a stabilization state, this button will end the stabilization time and set the GC to ready.

Temp Zones Status Display

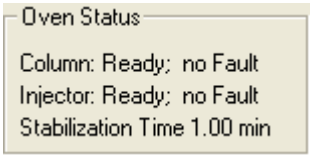


The temperature zones status display is in the middle portion of the 431-GC Status and Control window. The display includes the setpoints and actual temperatures of the column oven, and the injector of the 431-GC. The display is “Fault” if a fault occurs in the zone component or “Off” if the zone oven is off.

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.

Item	Description
Col Oven Setpoint	Abient+5 °C to 450 °C Displays the column oven programmed temperature setting in the active method.
Col Oven Actual	Abient+5 °C to 450 °C Displays the actual temperature of the column oven at the 431-GC
1177 Setpoint	50 to 450 °C Displays the 1177 injector oven programmed temperature setting in the active method.
1177 Actual	50 to 450 °C Displays the actual temperature of the 1177 injector oven at the 450-GC.

Oven Status Display

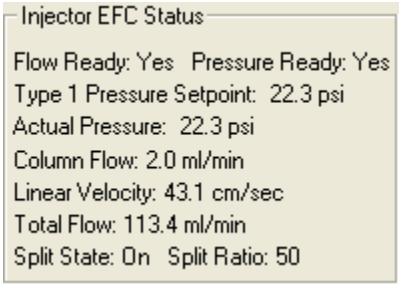


Oven Parameters:

Item	Description
Column Ready	Yes or No. The column oven is Ready (Yes) if the setpoints have been achieved and stabilized. The column oven is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the oven 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.
Column Fault	Yes or No. Displays if a fault in the column oven component has occurred.
Injector Ready	Yes or No. The injector oven is Ready (Yes) if the setpoints have been achieved and stabilized. The injector oven is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the injector becomes not ready or goes “out of tolerance”. .
Injector Fault	Yes or No. Displays if a fault in the injector oven component has occurred.

Item	Description
Stabilization Time	0.00 - 10.00 min Shows the 431-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.

Injector EFC Status Display



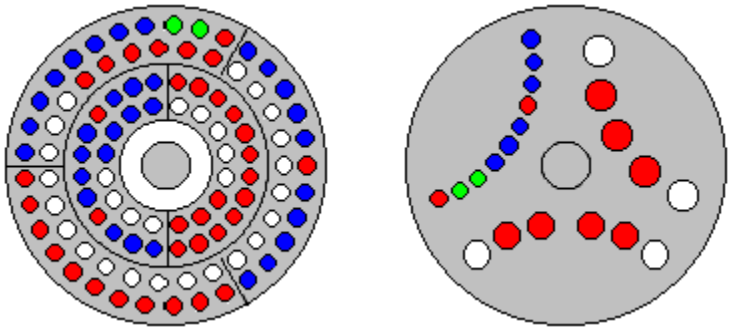
Injector EFC Status:

Item	Description
Flow Ready	Yes or No. The Type 21 Injector EFC component is Ready (Yes) if the setpoints have been achieved and stabilized. The Type 21 Injector EFC component is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the EFC 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.
Pressure Ready	Yes or No. The Type 21 Injector EFC component is Ready (Yes) if the setpoints have been achieved and stabilized. The Type 21 Injector EFC component is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the EFC 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.
Type 21 Pressure Setpoint	0.1 - 100 psi Displays the programmed column head pressure setting in the active method.
Actual Pressure	0.1 - 100 psi Displays the actual column head pressure at the 431-GC.
Column Flow	Displays, 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).

Item	Description
Linear Velocity	Displays, 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	Displays, in ml/min, the total flow rate through the system.
Split State	On or Off. Displays the current split state of the 1177 injector method.
Split Ratio	1 - 10000 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.

8400/8410 Carousel Display

When an 8400 AutoSampler or 8410 AutoInjector is connected to your 431-GC, the Carousel display will be visible in the 431-GC Status and Control window.



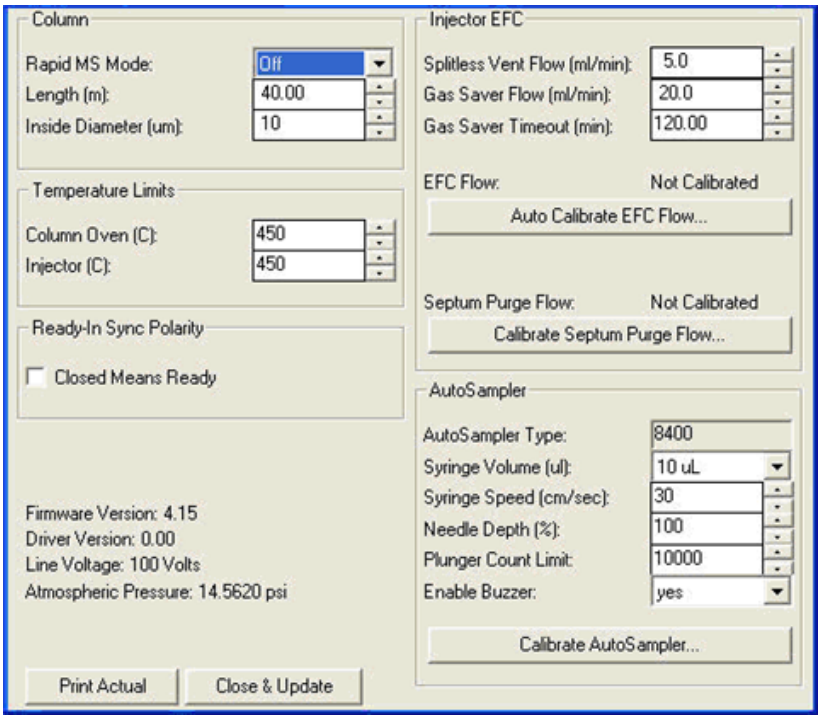
8400 AutoSampler Carousel / 8410 AutoInjector Carousel

Item	Description
Red fill	Indicates vials listed in the active SampleList that have not yet been sampled or are missing.
Green fill	Indicates the vial (vials in Dual Mode) currently being sampled.
Blue fill	Indicates the vials in the active SampleList that have been sampled.

Action	Description
Click a vial position	Displays the vial number for that position for 5 seconds.
Double-click a vial position	Opens the Inject Single Sample dialog box to inject a single sample.

431-GC Setup Dialog Box

This dialog box shows the hardware configuration reported by the 431-GC. This configuration is compared to and must match the configuration in the Method when it is activated. It also allows the configuration of the 431-GC to be changed from MS Workstation.



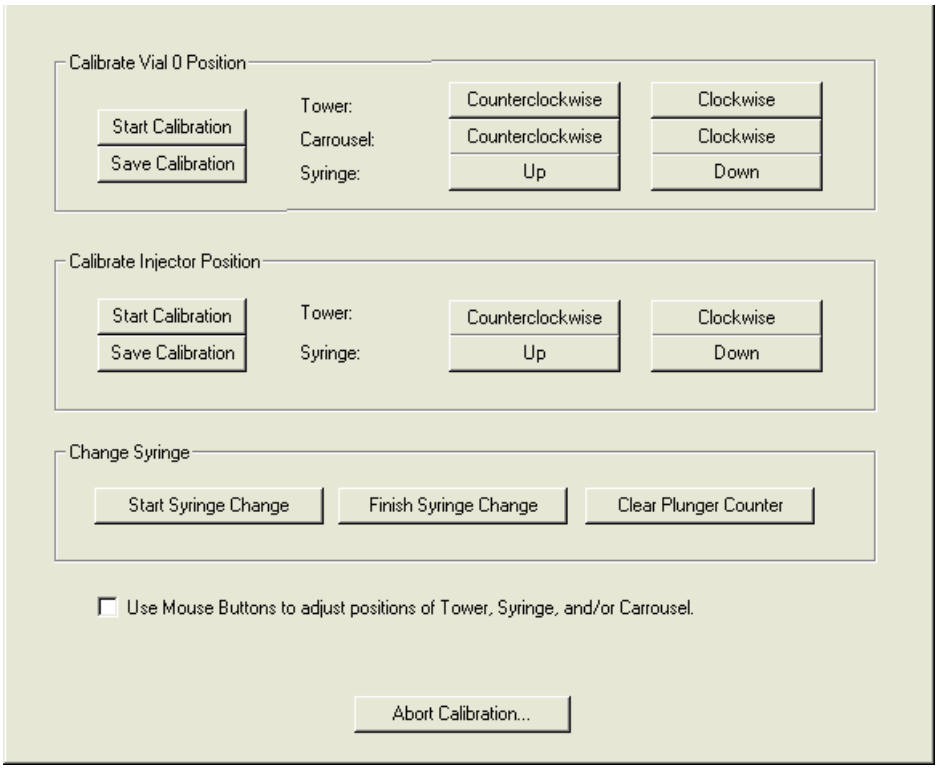
Item	Description
Column, Rapid MS Mode	On/Off When a Rapid-MS column is used in the 431-GC, the Rapid-MS Mode should be set to On. This will configure the GC to set the proper parameters for the Rapid-MS column. The column length and inside diameter entries will be grayed out.
Column, Length	The length of the column in meters. Values range from 0 to 250 meters.
Column, Inside Diameter	Inside diameter of the column in micrometers. Values range from 0 to 999 micrometers.
Temperature Limit, Column Oven	Upper temperature limit of the column oven. Values range from 50 to 450°C.
Temperature Limit, Injector	Upper temperature limit of the injector. Values range from 50 to 450°C.
Ready-In Sync Polarity	Is Ready-In a closed contact (Checked/Un-checked). Allows you to specify what switch state corresponds to External Device Ready.
Injector EFC, Splitless Vent Flow	The flow the system will vent when the split valve is left closed for the duration of the run

Item	Description
	such as during an on-column injection. This flow is diverted before the injector and thus does not influence the splitless nature of the run. This entry is ignored during split and splitless runs in which the split vent is opened.
Injector EFC, Gas Saver Flow	The lowest system flow rate that will be maintained during the gas saver period. This has a range of 1-100 mL/min and defaults to 20 mL/min.
Injector EFC, Gas Saver Timeout	A non-zero value entered for this parameter will cause the system to initiate a timer once a method is activated. If no system actions such as a run start or another method activation occurs before the Gas Saver Timeout is reached, then the system will reduce the flow through the system to the Gas Saver Flow. A method activation action will clear the Gas Saver Flow and bring the system to Ready for subsequent injections. A zero value entered for the Gas Saver Timeout will cause the Gas Saver Flow to be ignored and no Gas Saver actions will be performed.
Injector EFC, Auto Calibrate EFC Flow	Automatically calibrate the EFC system. When it is finished, the screen will display either a successful completion or detected problem message. No other GC functions can be performed during AutoCalibration. Note that AutoCalibration should be done on a semiannual basis.
Injector EFC, Calibrate Septum Purge Flow	Calibrate the septum purge. After installing a new column, the septum purge should be calibrated. Set the desired column head pressure. Then measure the actual septum purge flow rate and enter this value in the septum purge field. The septum purge flow rate is adjustable but is typically set at 3 - 5 mL/min.
Septum Purge Calibration, Desired Head Pressure	The desired column head pressure in psi. Range is 0.1 - 100 psi.
Septum Purge Calibration, Measured Flow Rate	The septum purge flow rate is adjustable but is typically set at 3 - 5 mL/min.
Print Actual	Sends the 431-GC setup parameters to the default printer.
Close & Update	Saves the changed parameters and reinitialize the 431-GC with the new parameters.
AutoSampler, Type	None, 8400, 8410 Displays the type of autosampler that is connected to the 431-GC.
AutoSampler, Syringe Volume	5 μL, 10 μL and 100 μL. Enter the syringe volume you will install and

Item	Description
	use with your CP-8400/8410. The 431-GC will use this value to set the correct entry selections and any needed internal settings to correctly use the indicated syringe size. Incorrectly setting this parameter may cause poor operation but will not harm either the GC or the AutoSampler.
AutoSampler, Syringe Speed	1 to 30 (cm/sec), default=30 The Injector Injection Speed parameters define the rate at which the needle will penetrate the injector septum and descend to the set Injector Needle Depth.
AutoSampler, Needle Depth	0 to 100, default=100 The Injector Needle Depth parameters define how far into the designated injector the needle will penetrate. 100% causes the needle to be completely inserted to its 2-inch length.
AutoSampler, Plunger Count Limit	(1-100,000) – This parameter defines the expected number of strokes the plunger is expected to survive without significant degradation. Once the entered value is exceeded, a message will be displayed on the CP-8400/8410 Status page indicating the plunger counter has exceeded the set value. The default number of strokes is 10,000.
AutoSampler, Enable Buzzer	*Buzzer at Start of Cycle* (On/Off) – A sound will be generated to warn of impending tower movements when this parameter is set to On. The default value is On.
AutoSampler, Calibrate AutoSampler	Displays the 8400/8410 AutoSampler Calibration Dialog Box.

Calibrate Autosampler Dialog Box

This dialog box helps the user to calibrate the 8400/8410 AutoSampler. Items that are not available are "grayed" in the actual screen.



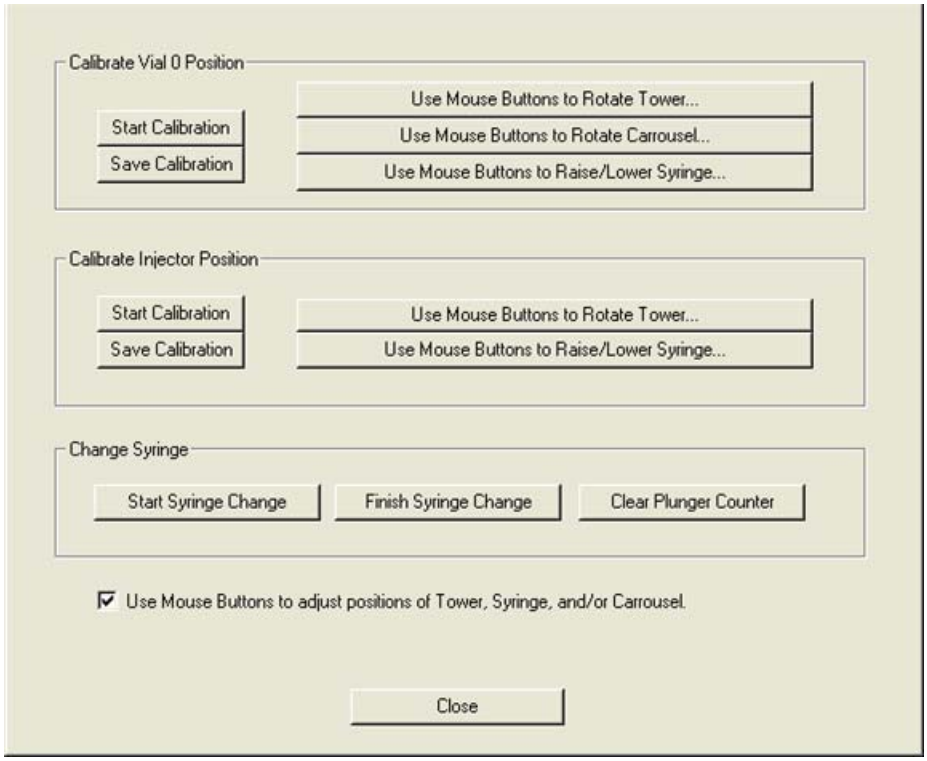
Item	Description
Calibrate Vial 0 Position, Start Calibration	To start the Vial 0 (or Vial 1) calibration, make certain a vial with the same form factor and cap as the ones you will be using for your analyses is placed in the 0 position of the carousel (or the Vial 1 position of the CP-8410). Press the Start Calibration button. Calibrating the Vial 0 (or Vial 1) position involves manipulating the positions of three different components. The object of the calibration is to position the syringe exactly over the center of the sampling target area of the vial. Upon starting the calibration procedure, the CP-8400/8410 will rotate the tower, rotate the carousel, and lower the syringe sled to the approximate location of Vial 0 (or Vial 1 if CP-8410). After the CP-8400/8410 has found the approximate Vial 0 (or Vial 1) position, visually check that the syringe sled is not resting on the vial top. If it is use the Syringe Up button. Press the button until the syringe sled is clear of the vial top by approximately 1 mm. Start the calibration process by adjusting the tower position
Calibrate Vial 0 Position, Save Calibration	When you have completed the Vial 0 (or Vial 1) calibration, press the Save Calibration button.
Calibrate Vial 0 Position, Tower Counterclockwise	Moves the tower 10 steps in the counterclockwise direction each time the button is pressed.

Item	Description
	NOTE: One basic rule associated with this calibration concerns rotation of the tower and carousel; to assure consistent operation, always approach the final calibration position with clockwise movements. To help facilitate this rule, the carousel will backup 10 steps when a counterclockwise action is selected but will move one step when a clockwise tower rotation is selected.
Calibrate Vial 0 Position, Tower Clockwise	Moves the tower 1 step in the clockwise direction each time the button is pressed. NOTE: One basic rule associated with this calibration concerns rotation of the tower and carousel; to assure consistent operation, always approach the final calibration position with clockwise movements. To help facilitate this rule, the carousel will backup 10 steps when a counterclockwise action is selected but will move one step when a clockwise tower rotation is selected.
Calibrate Vial 0 Position, Carousel Counterclockwise	Moves the carousel 10 steps in the counterclockwise direction each time the button is pressed. NOTE: One basic rule associated with this calibration concerns rotation of the tower and carousel; to assure consistent operation, always approach the final calibration position with clockwise movements. To help facilitate this rule, the carousel will backup 10 steps when a counterclockwise action is selected but will move one step when a clockwise tower rotation is selected.
Calibrate Vial 0 Position, Carousel Clockwise	Moves the carousel 1 step in the clockwise direction each time the button is pressed. NOTE: One basic rule associated with this calibration concerns rotation of the tower and carousel; to assure consistent operation, always approach the final calibration position with clockwise movements. To help facilitate this rule, the carousel will backup 10 steps when a counterclockwise action is selected but will move one step when a clockwise tower rotation is selected.
Calibrate Vial 0 Position, Syringe Up	Use the Syringe Up button and adjust the syringe sled height so that the needle is just barely above the vial cap (You should be able to see about a paper's thickness of space between the syringe sled needle guide and the top of the vial cap. The penetration depth into the vial is measured from the bottom of the needle guide, so this height will give you optimum penetration depth.).
Calibrate Vial 0 Position, Syringe Down	Use the Syringe Down button and adjust the syringe sled height so that the needle is just barely above the vial cap (You should be able to see about a paper's thickness of space

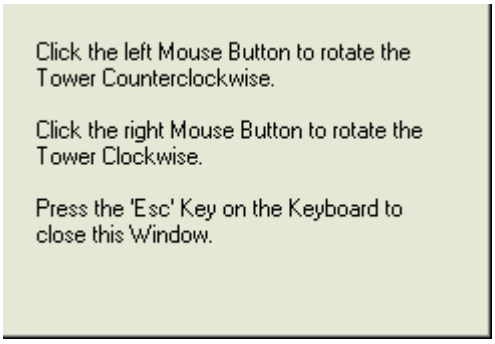
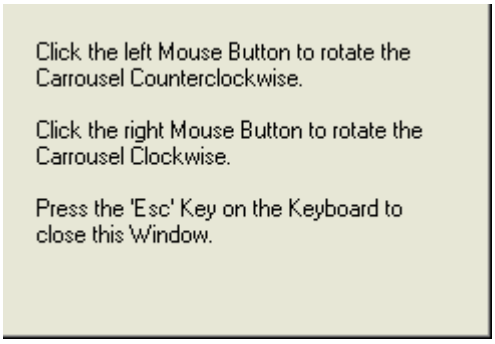
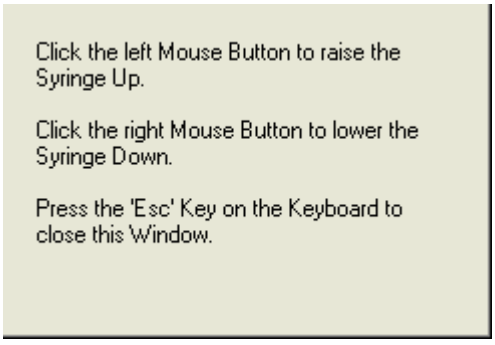
Item	Description
	between the syringe sled needle guide and the top of the vial cap. The penetration depth into the vial is measured from the bottom of the needle guide, so this height will give you optimum penetration depth.).
Calibrate Injector Position, Start Calibration	Press the Start Calibration. The CP-8400/8410 will rotate the tower so that it is over the Injector position and lower the syringe sled so that it is over the injector. If the needle guide descends so that it is either resting on the inject switch or below the needle cone on the inject switch, use the Syringe Up button and move the sled up until the needle guide is just above the injector cone.
Calibrate Injector Position, Save Calibration	Press the Save Calibration softkey when the Injector calibration is complete.
Calibrate Injector Position, Tower Counterclockwise	Using the Tower Counterclockwise button rotates the tower counterclockwise 10 steps. Position the tower directly over the injector Inject Switch Locator cone.
Calibrate Injector Position, Tower Clockwise	Using the Tower Clockwise button rotates the tower clockwise 1 step. Position the tower directly over the injector Inject Switch Locator cone.
Calibrate Injector Position, Syringe Up	Using the Syringe Up button adjust the height of the needle guide such that the sled is just resting on or very slightly depressing the Injector Switch and is covering the locator cone.
Calibrate Injector Position, Syringe Down	Using the Syringe Down button adjust the height of the needle guide such that the sled is just resting on or very slightly depressing the Injector Switch and is covering the locator cone.
Change Syringe, Start Syringe Change	Selecting Start Syringe Change will cause the tower to rotate such that the user will have easy access to the syringe for routine service and syringe removal and replacement. The buzzer will sound before any tower movement occurs. Press the Finish Syringe Change softkey upon completion of the syringe maintenance.
Change Syringe, Finish Syringe Change	Selecting Finish Syringe Change will cause the tower to return to its previous position and state. The buzzer will sound prior to movement as designated by the “Buzzer at start of cycle” setting.
Change Syringe, Clear Plunger Counter	Selecting this softkey causes the Plunger stroke count to be reset to 0.
Use Mouse Buttons to adjust positions of Tower, Syringe, and/or Carousel	Checking this box, changes the Calibrate AutoSampler Dialog Box for the positions to be adjusted with the mouse.
Close	Closes the dialog box.

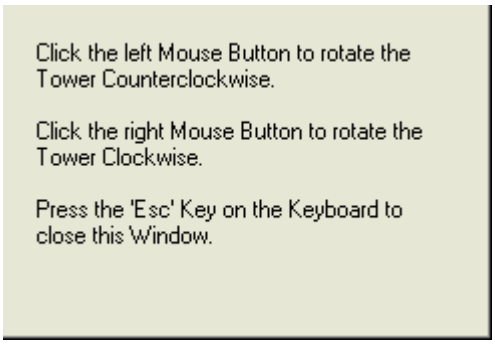
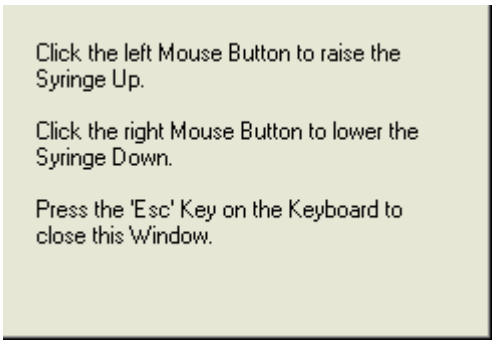
Use Mouse Buttons to Adjust Positions

The following information is displayed in the Calibrate Autosampler dialog box when you click this box.



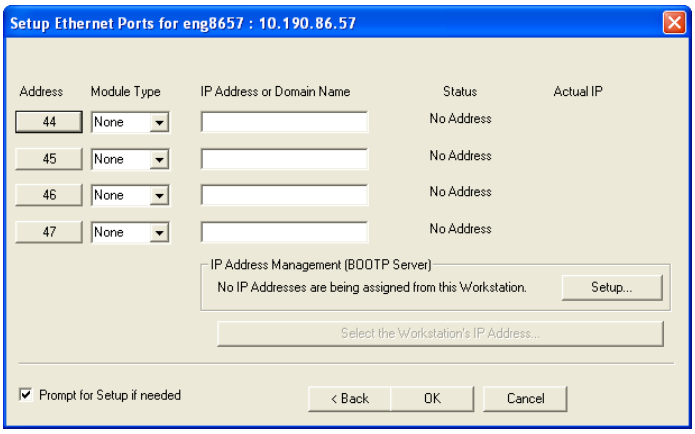
Item	Description
Calibrate Vial 0 Position, Start Calibration	To start the Vial 0 (or Vial 1) calibration, make certain a vial with the same form factor and cap as the ones you will be using for your analyses is placed in the 0 position of the carousel (or the Vial 1 position of the CP-8410). Press the Start Calibration button. Calibrating the Vial 0 (or Vial 1) position involves manipulating the positions of three different components. The object of the calibration is to position the syringe exactly over the center of the sampling target area of the vial. Upon starting the calibration procedure, the CP-8400/8410 will rotate the tower, rotate the carousel, and lower the syringe sled to the approximate location of Vial 0 (or Vial 1 if CP-8410). After the CP-8400/8410 has found the approximate Vial 0 (or Vial 1) position, visually check that the syringe sled is not resting on the vial top. If it is use the Syringe Up button. Press the button until the syringe sled is clear of the vial top by approximately 1 mm. Start the calibration process by adjusting the tower position

Item	Description
Calibrate Vial 0 Position, Save Calibration	When you have completed the Vial 0 (or Vial 1) calibration, press the Save Calibration button.
Calibrate Vial 0 Position, Use Mouse Buttons to Rotate Tower	Clicking this button will display the Rotate Tower dialog box. 
Calibrate Vial 0 Position, Use Mouse Buttons to Rotate Carousel	Clicking this button will display the Rotate Carousel dialog box. 
Calibrate Vial 0 Position, Use Mouse Buttons to Raise/Lower Syringe	Clicking this button will display the Raise/Lower Syringe dialog box. 
Calibrate Injector Position, Start Calibration	Press the Start Calibration. The CP-8400/8410 will rotate the tower so that it is over the Injector position and lower the syringe sled so that it is over the injector. If the needle guide descends so that it is either resting on the inject switch or below the needle cone on the inject switch, use the Syringe Up button and move the sled up until the needle guide is just above the injector cone.

Item	Description
Calibrate Injector Position, Save Calibration	Press the Save Calibration softkey when the Injector calibration is complete.
Calibrate Injector Position, Use Mouse Buttons to Rotate Tower	Position the tower directly over the injector Inject Switch Locator cone. Clicking this button will display the Rotate Tower dialog box. 
Calibrate Injector Position, Use Mouse Buttons to Raise/Lower Syringe	Using the Syringe Up button adjust the height of the needle guide such that the sled is just resting on or very slightly depressing the Injector Switch and is covering the locator cone. Clicking this button will display the Raise/Lower Syringe dialog box. 
Change Syringe, Start Syringe Change	Selecting Start Syringe Change will cause the tower to rotate such that the user will have easy access to the syringe for routine service and syringe removal and replacement. The buzzer will sound before any tower movement occurs. Press the Finish Syringe Change softkey upon completion of the syringe maintenance.
Change Syringe, Finish Syringe Change	Selecting Finish Syringe Change will cause the tower to return to its previous position and state. The buzzer will sound prior to movement as designated by the “Buzzer at start of cycle” setting.
Change Syringe, Clear Plunger Counter	Selecting this softkey causes the Plunger stroke count to be reset to 0.
Use Mouse Buttons to adjust positions of Tower, Syringe, and/or Carousel	Un-checking this box, changes the Calibrate AutoSampler Dialog Box for the positions to be adjusted with the buttons on the screen.
Close	Closes the dialog box.

Setup Ethernet Ports Dialog Box

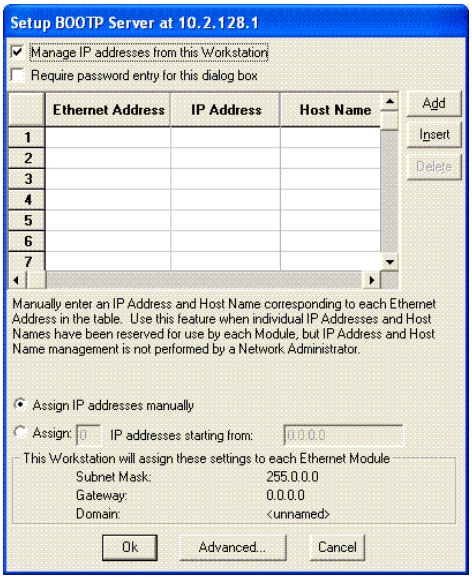
This dialog box is displayed the first time that Workstation guides you through the setup of your 431-GC in System Control. This dialog box is also accessed from the Instrument/Setup Ethernet Communications menu item of System Control.



Item	Description	
Address	44, 45, 46, or 47 Click the Address button to attach to a 431-GC on the Ethernet network. If you are running on a company network, only GCs on the same local subnet appear in the Select Available Modules dialog box that is displayed after clicking the Address button.	
Module Type	None or 431-GC This field is set if you select a 431-GC using the Address button. If you specify an IP Address or Domain Name explicitly, then select 431-GC from this combobox.	
IP Address or Domain Name	This field is set if you select a 431-GC using the Address button. To connect to a GC in a different subnet, type its IP Address directly into the IP Address or Domain Name field.	
Status	Available, Online, In Use By <client>, Not Responding, or No Address Displays the connection status of the 431-GC.	
	Status	**Meaning**
	Available Online In Use By <client> Not Responding No Address	Not in use by anyone In use by this Workstation In use by another Workstation Not responding to Workstation queries No IP Address or name specified
Actual IP	Displays the actual IP address of the connected 431-GC.	
Setup...	Click to setup IP address management (BOOTP Server). The Setup BOOTP Server Dialog Box is displayed.	

Setup BOOTP Server Dialog Box

If IP addresses are managed by a Network Administrator from a central source, the 431-GCs must be added to the list of devices requiring IP addresses. IP addresses must be assigned to GCs using a BOOTP Server. A BOOTP Server lists Ethernet addresses (which are unique to each communication card installed in each 431-GC) along with the IP addresses that are to be assigned to the corresponding device. You may obtain the Ethernet address for each GC from the GC's front panel. Turn on the 431-GC and press any key to allow it to start in local mode.

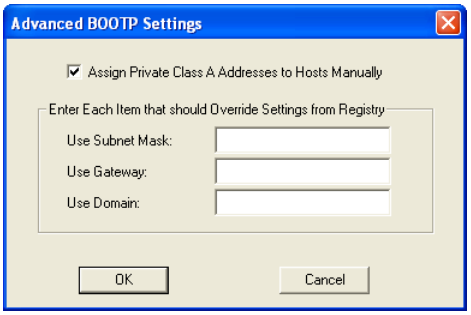


Item	Description
Manage IP addresses from this Workstation	Checked or not checked When IP addresses are managed from a central location by a Network Administrator, the BOOTP Server on your Workstation must be disabled (not checked).
Require password entry for this dialog box	Checked or not checked Check this box to restrict access to the BOOTP Server dialog box to avoid inadvertent or unauthorized changes to IP address assignments. If this item is checked, the next time you enter the BOOTP Server dialog box, you will be prompted for a password. The initial password is blank (no password). To set your password initially, enter the desired password in the Enter new password and Re-enter new password fields. Subsequent entry into the BOOTP Server will require this password.
Ethernet Address	Displays the Ethernet address of any 431-GCs already connected to the network and powered on. You may also manually enter an Ethernet address for a 431-GC.

Item	Description
IP Address	Displays the IP address of any 431-GCs already connected to the network and powered on. You may also manually enter an IP address for a 431-GC. Use the manual entry of IP addresses and Host Names when individual IP addresses have been reserved for use by each 431-GC but IP Address and Host Name management is not performed by a Network Administrator.
Host Name	You must enter a name for each 431-GC. The IP address will not be assigned to the GC until a name is entered.
Assign IP addresses manually	Selected or not selected Select this entry if you manually enter IP addresses and Host Name entries in the table.
Assign IP addresses starting from	Selected or not selected Select this entry to consecutively assign IP addresses beginning from a particular address. Enter the number of IP addresses to assign automatically and the starting IP address. As 431-GCs are powered on, IP addresses are automatically assigned from the specified address.
Subnet Mask	Displays the subnet mask assigned to the Workstation. This parameter is assigned in the TCP/IP network setup in the Control Panel application.
Gateway	Displays the Gateway assigned to the Workstation. This parameter is assigned in the TCP/IP network setup in the Control Panel application.
Domain	Displays the Domain name assigned to the Workstation. This parameter is assigned in the TCP/IP network setup in the Control Panel application.

Advanced BOOTP Settings Dialog Box

This dialog lets you enter advanced settings.



Item	Description
Assign Private Class A addresses to Hosts Manually	Checked or not checked Determines if IP addresses are entered in the Setup BOOTP Server dialog box (checked) or if they are generated (unchecked).
Use Subnet Mask	Enter the subnet mask here. This is only used when the Manage IP addresses from this Workstation checkbox is checked in the Setup BOOTP Server dialog box.
Use Gateway	Enter the gateway address here. This is only used when the Manage IP addresses from this Workstation checkbox is checked in the Setup BOOTP Server dialog box.
Use Domain	Enter the domain name here. This is only used when the Manage IP addresses from this Workstation checkbox is checked in the Setup BOOTP Server dialog box.

Method Builder Menus

File Menu

Menu Item	Description
New	Starts the Method Builder dialog to aid and guide you through creating the Method sections that you need for an instrument connected to Varian MS Workstation.
Open...	Opens an existing Method file to edit. Opens the Open Method File Dialog Box.
Close	Closes the currently selected Method.
Save	Saves the current settings under the name of the current Method file.
Save As...	Saves a Method under a new name. Opens the Save Method File As Dialog Box
Set Password	Opens the Add Password Dialog Box or the Change Password Dialog Box.
Prompt for Action at Startup	Enables (checked) or disables (unchecked) the Create/Open Method File dialog box when Method Builder is started.
Print…	Prints one or more sections from the current Method.
Print Preview	Allows user to view any or all sections of the Method in printer format prior to printing.
Print Setup...	Sets preferences for printing. Opens the Printer Setup Dialog Box.
Add Module Control…	Starts the Method Builder dialog to aid and guide you through creating the Method sections that you need for an instrument connected to a Varian MS Workstation.
Add Post-run Processing…	Starts the Method Builder dialog at the start of the Post-run Processing section to aid and guide you through creating the data handling and printing method sections.
Delete Section	Opens the Delete Method Sections Dialog Box listing the sections of the Method. Highlight the sections to be deleted and click on the Delete button.
Import Section...	Imports (copies) Method sections from another Method into the current Method. Used to create a new Method with some of the settings from another Method. Opens the Import Method File, File Sections Dialog Box.
Recent Files List	This is a section of the File menu that lists the previously opened Method files for quick access.
Exit	Closes Method Builder. If you have made any changes to the Method, you are prompted to save the changes before closing Method Builder.

Edit Menu

Menu Item	Description
Undo	Undoes the last edit to an item. If the last edit cannot be undone, this menu item is disabled (grayed).
Cut	Copies selected items to the clipboard and removes them from the Method.
Copy	Copies selected items to the clipboard.
Paste	Pastes the clipboard contents to the selected item.
Delete	Deletes selected items. If a Method section is selected, the Delete Method Sections Dialog Box is opened..
Fill Down	Replicates the first selected table line to the other selected table lines.

View Menu

Menu Item	Description
Toolbar	When checked, the Main Toolbar is displayed.
Window Toolbar	When checked, the Window Toolbar is displayed.
Directory Toolbar	When checked, the Directory Toolbar is displayed.
Status Bar	When checked, the Status bar at the bottom of the Method Builder window is displayed.
Method Directory	When checked, the Window Toolbar pane is displayed. This pane provides a tree-structured view of the Method and allows mouse click selection of Method sections.

Window Menu

Menu Item	Description
New Window	Opens a second window into the same Method. This is useful for setting up side by side comparisons of different Method sections.
Cascade	Arranges the open Method Windows in a cascaded format for easy switching between multiple Methods and sections.
Tile Vertically	Tiles the open Method Windows vertically (side by side).
Tile Horizontally	Tiles the open Method Windows horizontally (one above the other).
Arrange Icons	Arranges iconized Method Windows along the bottom of the Method Builder Window.
Next Pane	Switches between The Window Toolbar pane and The Method Builder Window pane.

Menu Item	Description
Open Window List	A list of the currently open Method Builder windows. Provides quick access to windows that are hidden behind other windows.

Help Menu

Menu Item	Description
Help Topics	Displays the help you are now viewing.
Product Support Web Site	If you have Internet access and a web browser installed on your computer, this option will automatically open the Varian, Inc. Web Site. Here you will find the latest software and documentation updates for the Varian, Inc. suite of products, along with additional notes, tips, and answers to frequently asked questions. You may wish to visit this site periodically to see if new information is available that may be pertinent to you.
About Method Builder	Displays the About Box for the Method Builder application. The About Box contains information about the software version, installation information, and a list of the instrument control modules that you have installed.

Method Builder Toolbars

Overview

There are three toolbars on the main window: the Main Toolbar, the Directory Toolbar, and the Window Toolbar. The Main Toolbar can be used to open, save, or print Method files; the Directory Toolbar is used to traverse the Method Directory pane; and the Window Toolbar is used to position the Method windows. By clicking an area of the toolbar between buttons, each toolbar can be dragged with the left mouse button to a docked location along any side of the Method Builder main window, or positioned independently anywhere on the screen. In addition, each toolbar can be hidden or closed. If the toolbar is hidden, it may be displayed by selecting the appropriate menu item from the View menu of Method Builder.

Main Toolbar

	Starts the Method Builder dialog to aid and guide you through creating the Method sections that you need for an instrument connected to a Varian MS Workstation.
	Opens an existing Method file to edit. Opens the Open Method File Dialog Box.
	Saves the current settings under the name of the current Method file.
	Saves a Method under a new name. Opens the Save Method File As Dialog Box.
	Opens the Add Password Dialog Box or the Change Password Dialog Box.
	Starts the Method Builder dialog to aid and guide you through creating the Method sections that you need for an instrument connected to Varian MS Workstation.
	Starts the Method Builder dialog at the start of the Post-run Processing section to aid and guide you through creating the data handling and printing method sections.
	Opens the Delete Method Sections Dialog Box listing the sections of the Method. Highlight the sections to be deleted and click on the Delete button.
	Copies selected items to the clipboard and removes them from the Method.

	Copies selected items to the clipboard.
	Pastes the clipboard contents to the selected item.
	Deletes selected items. If a Method section is selected in the Method Directory pane, the Delete Method Sections dialog box is opened..
	Replicates the first selected table line to the other selected table lines.
	Prints one or more sections from the current Method.
	Displays the help you are now viewing.

Directory Toolbar

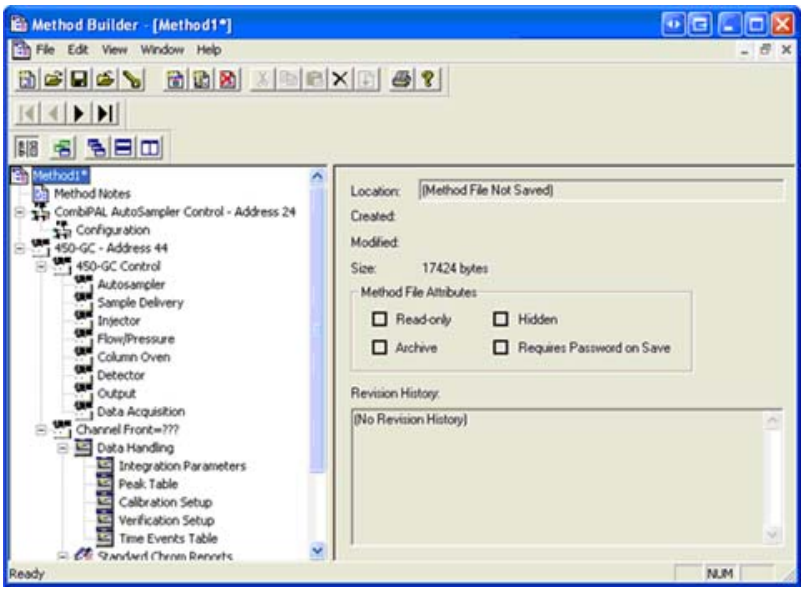
	From the current selection in the Method Directory pane, selects the previous directory item that is a collapsible / expandable branch. The displayed Method Parameters pane is used to reassign Varian MS Workstation bus addresses for hardware modules and to reassign channels for post-run processing of detector module data. The module Method sections can also be accessed from the displayed Method Parameters pane.
	From the current selection in the Method Directory pane, selects the previous directory item that is a Method Parameters window for a section in the Method file. Pressing this toolbar button will step backward from the current selection through each section of the open Method.
	From the current selection in the Method Directory pane, selects the next directory item that is a Method Parameters window for a section in the Method file. Pressing this toolbar button will step forward from the current selection through section of the open Method.
	From the current selection in the Method Directory pane, selects the next directory item that is a collapsible / expandable branch. The displayed Method Parameters pane is used to reassign Varian MS Workstation bus addresses for hardware modules and to reassign channels for post-run processing of detector module data. The module Method sections can also be accessed from the displayed Method Parameters pane.

Window Toolbar

	When pressed, the RecalcList Generation Dialog Box pane is displayed. This pane provides a tree-structured view of the Method and allows mouse click selection of Method sections. This toolbar button toggles to show or hide the Method Directory pane.
	Opens a second window into the same Method. This is useful for setting up side by side comparisons of the same or different Method sections.
	Arranges the open Method Windows in a cascaded format for easy switching between multiple Methods and sections.
	Tiles the open Method Windows horizontally (one above the other).
	Tiles the open Method Windows vertically (side by side).

Method Builder Window

Overview



The Method is displayed in a window that is split into a left and a right pane. The left pane is the Method Directory pane and provides a tree-structured view of the Method. The right pane is the Method Parameters pane and provides the capability to configure various method parameters. The items displayed in the Method Parameters pane correspond to the selected item in the Method Directory pane.

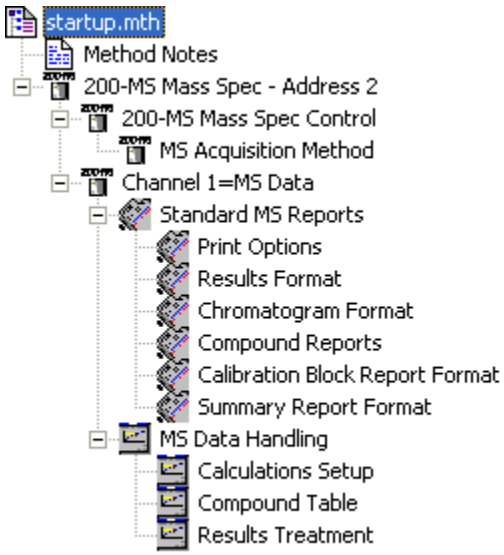
The splitter bar that separates the panes is used to size the panes. When the mouse cursor is over the splitter bar, click and drag the mouse to size the area displayed in each pane. You can also hide the Method Directory (or left) pane by clicking the Hide Directory toolbar button on the Window toolbar.

By default, the toolbar buttons are arranged at the top of the main window below the Method Builder menu. There are three toolbars: the Main toolbar for opening, saving, and printing Method files; the Directory toolbar for traversing the tree displayed in the Method Directory pane; and the Window toolbar for positioning the Method windows. By positioning the mouse cursor over a toolbar button, a short description of it is displayed for a brief time. In addition, a status bar is displayed at the bottom of the Method Builder main window. Any of the toolbars and the status bar may be hidden or displayed by selecting the appropriate item from the Method Builder View menu.

Only one instance of the Method Builder application is used to display and edit Method files. If the Method Builder application is already running when you

choose to edit a Method file, a new window is displayed for the Method file. Any previously open Method file can be accessed by selecting the appropriate window from the Window menu. In addition, if you open another Method file from the File menu of Method Builder, the Method file is displayed in a new window; any previously open Method file is not closed. From the Window menu or using the Window toolbar, the Method file windows can be selected, cascaded, or tiled in order to compare the same sections in different Method files.

Method Directory



The Method file is displayed in the Method Directory pane as a tree-structured view of the Method consisting of items that can be expanded in further detail (a "+" or "-" is displayed to the left of the labeled icon) and items that cannot be further expanded in the tree (no "+" or "-" appears to the left of the labeled icon). The top-most item in the tree is the name of the Method file. An asterisk (*) follows the name if the Method file has been modified since it was opened or last saved. The Method Notes are always displayed as a branch below the Method file name. All of the next level of branches of the directory tree represent hardware module components (detectors, pumps, etc.). The hardware modules are listed in ascending order of their addresses on the Varian MS Workstation bus.

If the hardware module is a detector component, then the branch for that module is expanded into the control method for the detector and a branch for each channel of the detector. The branches for the control method represent the groups of editable parameters for detector control and data acquisition by the detector. The branches for the channels are expanded into the post-run processing applications that can be applied to the channels. For each post-run application, the branch for that application is expanded into the groups of editable parameters for the application.

If the hardware module is not a detector component, then the branch for that module is expanded into the groups of editable parameters for the control method of that module.

If a minus (-) sign is displayed to the left of the name in the directory tree, then

that branch in the tree can be collapsed by either clicking the minus sign or by pressing the minus key on the keyboard. If a branch is collapsed, then a plus (+) sign is displayed to the left of the name in the directory tree. Clicking the plus sign or pressing the plus key on the keyboard expands that branch of the tree. You may also double-click the name of the branch in order to expand or collapse the branch.

Clicking on an item in the Method Directory pane will display the corresponding parameters for that selection in the Method Parameters (or right) pane. For example, clicking “Method Notes” in the Method Directory pane will display the Method notes for the Method file in the right pane.

Method Parameters

The Method Parameters pane displays the corresponding item of the Method Directory tree selected in the Method Directory pane. There are four types of windows that can be displayed in the Method Parameters pane: Method file information, Method Notes, hardware component section descriptions, and hardware component editable parameters.

If the Method file name is selected in the Method Directory (left) pane, then the Method Parameters (right) pane displays the file information. The Method file information includes the fully qualified path name of the file, creation and modification dates, file size, file attributes, and the Revision History of the Method file.

If “Method Notes” is selected in the Method Directory (left) pane, then the Method Parameters (right) pane displays the notes for the Method file as free-form text. The Method notes can include any information about the Method such as setup or how the Method is to be run. The Method notes are always printed with the Method.

For the low-level branches of a hardware component in the Method Directory tree (those that cannot be expanded), the Method Parameters pane displays editable parameters for controlling the hardware module and data acquisition, and for post-run processing of detector data.

For all other hardware component branches of the Method Directory tree, the Method Parameters pane displays a description of the Method sections associated with that hardware component branch. The user can reassign the bus address of a hardware module, reassign the bus address or channel for post-run processing, or select the particular group of processing or control parameters to edit. In addition, the time of last modification of the processing or control parameters is also listed. In the list containing the names of the Post-Run Processing Parameters or Method Control Parameters, double-click the list item in order to display the editable parameters. You may also select the name and press the ENTER or RETURN key on the keyboard in order to display the editable parameters for that list item. To reassign the address or channel for all of the listed Method Control or Post-Run Processing Parameters, select the new channel or address from the drop-down list in the Method Parameters pane. Any addresses or channels for which a Method section already exists are omitted from the drop-down lists.

Automation File Editor Command Reference

Menus

File Menu

Menu Item	Description
New	A sub-menu displays RecalcList, SampleList and Sequence. Selecting one of them displays the Create a New Automation File dialog box to name a new file of the selected type.
Open	A sub-menu displays RecalcList, SampleList and Sequence. Selecting one of them displays the Open an Automation File dialog box to open an existing automation file of the selected type .
Save	Saves the currently displayed automation file with the existing name.
Save As	Displays the Save Automation File As dialog box, allowing you to save the currently displayed automation file with a new name.
Print	Prints the currently displayed automation file.
Printer Setup	Opens the Print Setup Dialog Box to select a printer and set options for it. You can open the Print Setup dialog box from the System Control Printer Setup dialog box.
Exit	Quits the Automation File Editor. If any file is open and changes have not been saved, you will be prompted to do so.

Edit Menu

Menu Item	Description
Cut	Deletes a selection and copies it to the Clipboard. Used to remove or move a selected part of a spreadsheet.
Copy	Copies a selection to the Clipboard. Used to duplicate a selection and place the duplicate in a new place (using Paste).

Menu Item	Description
Paste	Inserts previously cut or copied information that was stored in the Clipboard into a spreadsheet.
Clear	Deletes a selection but leaves the Clipboard unchanged.
Add	Adds a new line in a Sequence, SampleList or RecalcList.
Insert	Inserts a new line in a Sequence, SampleList or RecalcList.
Select All	Selects all lines in a Sequence, SampleList or RecalcList.
Fill Down	Causes the contents of the top cell in a series of highlighted cells to be copied to the cells below it. Used to edit all the cells in a column quickly.
Edit Notes	Opens the Edit Notes dialog box to permit editing of the notes associated with the currently open automation file.

Help Menu

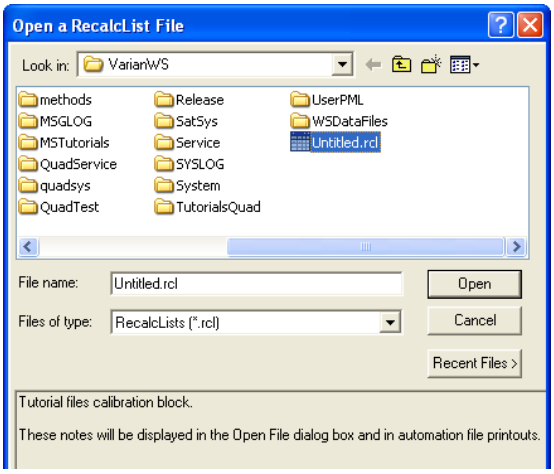
Menu Item	Description
Help Topics	Displays the help you are now viewing.
Product Support Web Site	If you have Internet access and a web browser installed on your computer, this option will automatically open the Varian MS Workstation Product Support Web Site. Here you will find the latest software and documentation updates for the Varian MS Workstation suite of products, along with additional notes, tips, and answers to frequently asked questions. You may wish to visit this site periodically to see if new information is available that may be pertinent to you.
About Automation File Editor	Displays the About Box for the Automation File Editor application. The About Box contains information about the software version, installation information, and a list of the instrument control modules that you have installed.

Main Toolbar

Item	Description
	A sub-menu displays RecalcList, SampleList and Sequence. Selecting one of them displays the Create a New Automation File dialog box to name a new file of the selected type.
	A sub-menu displays RecalcList, SampleList and Sequence. Selecting one of them displays the Open an Automation File dialog box to open an existing automation file of the selected type .
	Saves the currently displayed automation file with the existing name.
	Displays the Save Automation File As dialog box, allowing you to save the currently displayed automation file with a new name.
	Prints the currently displayed automation file.
	Deletes a selection and copies it to the Clipboard. Used to remove or move a selected part of a spreadsheet.
	Copies a selection to the Clipboard. Used to duplicate a selection and place the duplicate in a new place (using Paste).
	Inserts previously cut or copied information that was stored in the Clipboard into a spreadsheet.
	Causes the contents of the top cell in a series of highlighted cells to be copied to the cells below it. Used to edit all the cells in a column quickly.

Open Automation File Dialog Box

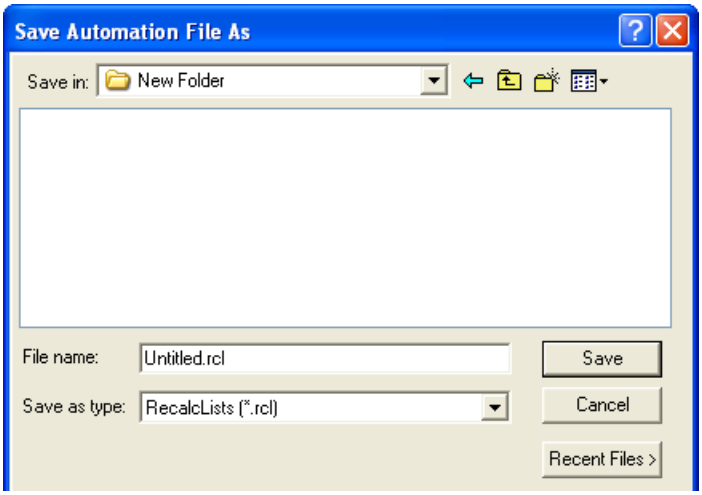
This dialog box is used to specify or open an automation file. The Open Automation File dialog box appears with several different titles, depending upon how you access it. In all cases, it contains the fields listed below in forms appropriate for the type of file you are about to open.



Item	Description
Look in	Lists the available folders and files. To see how the current folder fits in the hierarchy on your computer, click the down arrow. To see what's inside a folder, click it. The box below shows the folders and files in the selected location. You can also double-click a folder or file in that box to open it. To open the folder one level higher, click the “up arrow” button on the toolbar.
File list	Lists the folders and files in the selected location. To see what's inside a folder, double-click it. You can also use the Look In box to see the hierarchy of folders. To open the folder one level higher, click the “up arrow” button on the toolbar.
File name	Shows the currently selected file.
Files of type	Restricts the list of files to only those matching the selected type.
Recent Files	Click on this button to display a list of recently selected files. When you select a file from this list, its name is displayed in the File name box.
Notes	Displays any notes and/or revision log associated with the currently selected file.
Open	Opens the selected file.
Cancel	Cancels file selection.

Save Automation File As Dialog Box

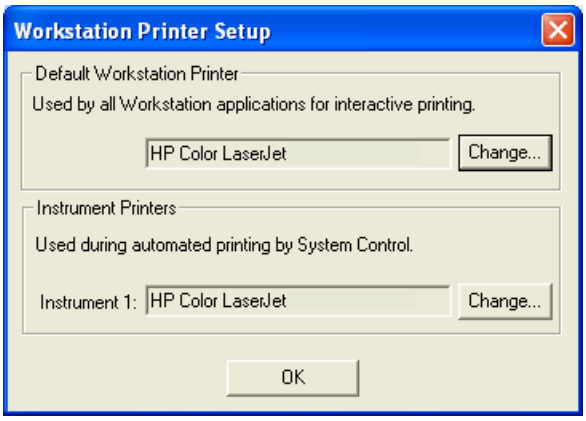
This dialog box is used to name an automation file. The Save Automation File As dialog box appears with several different titles, depending upon how you access it. In all cases, it contains the fields listed below in forms appropriate for the type of file you are about to save.



Item	Description
Save in	Lists the available folders and files. To see how the current folder fits in the hierarchy on your computer, click the down arrow. To see what's inside a folder, click it. The box below shows the folders and files in the selected location. You can also double-click a folder or file in that box to open it. To open the folder one level higher, click the “up arrow” button on the toolbar.
File list	Lists the folders and files in the selected location. To see what's inside a folder, double-click it. You can also use the Save In box to see the hierarchy of folders. To open the folder one level higher, click the “up arrow” button on the toolbar.
File name	Shows the currently specified file.
Save as type	Specifies the type of file to save.
Recent Files	Click on this button to display a list of recently selected files. When you select a file from this list, its name is displayed in the File name box.
Save	Saves the file with the specified name.
Cancel	Cancels file saving.

Print Setup Dialog Box

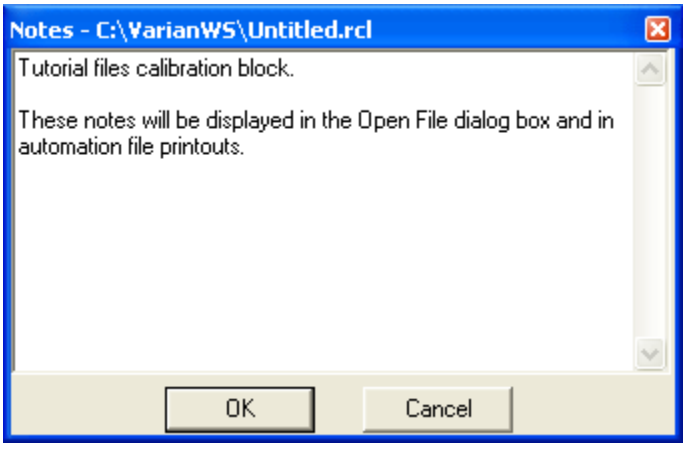
This dialog box is used to specify the printers that will be used by Varian MS Workstation applications both interactively and during automation.



Item	Description
Default MS Workstation Printer	Displays the printer that is used when printing interactively from Varian MS Workstation applications. Click on the Change button to select a different printer.
Instrument Printers	Displays the printer that is used when printing under automation from System Control. Since the Varian MS Workstation is a single instrument workstation, the printer specifications for instruments 2-4 will be ignored.

Edit Notes Dialog Box

This dialog box allows you to enter descriptive notes associated with an automation file. These notes can be viewed when selecting the file, and are included in the file's printout.

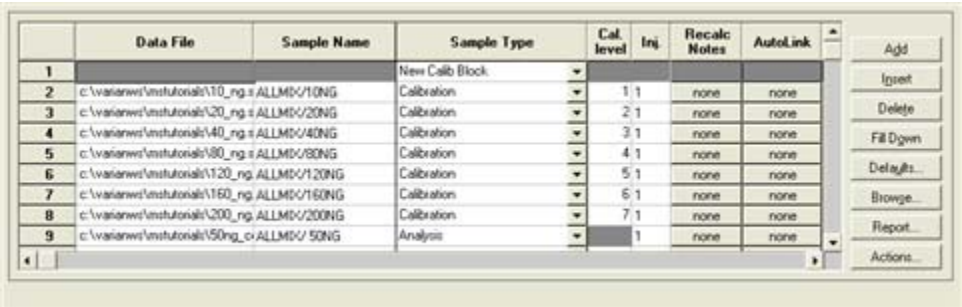


Item	Description
Notepad Area	Shows any notes attached to the file. The notes may describe the contents of the file, its uses, restrictions, etc. The Notepad Area is scrollable if the notes exceed the available space. The notes can be edited here, either by typing text directly, or by pasting text from the Clipboard by pressing the keys: CTRL V simultaneously.

RecalcList Window

Data Files can be added to a RecalcList by clicking on a cell in the Data File column and typing the file name, or by pressing the Browse... button and selecting the file name. Another way of quickly adding one or more Data Files to a RecalcList is by selecting the files of interest in the Explorer, and dragging them over the RecalcList Window. When you release the mouse button, the Data Files are automatically appended to the RecalcList.

Note that a Recalc List may contain standard GC data files (.run extension) as well as MS data files (.sms extension). Some of the Recalc List items described below are handled differently for the two data file types. When the list is processed, the appropriate data handling is used automatically for each data file.



Item	Description
Data File	Shows the name and path of the Data File for each sample.
Sample Name	Cannot be edited. Shows the name of each sample in the RecalcList.
Sample Type	Baseline, Analysis, Calibration, Verification, Print Calib, New Calib Block, AutoLink, Activate Method Sets the sample type, or automation action, of each line in the RecalcList.
Cal. Level	1 to 10 Sets the calibration level of each calibration or verification sample in the RecalcList.
Inj	Cannot be edited. Shows the number of injections made of each sample in the RecalcList.

Item	Description
Recalc Notes...	Up to 180 characters Opens the Notes window for the selected record to edit or create a note about the sample. This note is stored separately from the original injection notes.
AutoLink...	Two AutoLink commands when Sample Type is Baseline, Analysis, Calibration, or Verification. One AutoLink command when Sample Type is AutoLink. One Activate Method Command when Sample Type is Activate Method. Opens the AutoLink Parameters dialog box to set the options for linking to a remote application during automation through System Control. Opens the Activate Method Dialog Box to set the path name for activating a new method during automation of a RecalcList through System Control.
Unid Peak Factor	0 to 1,000,000.0 Sets a calibration factor for unidentified peaks. Not used by calibration samples.
Multiplier	0.000001 to 1,000,000.0 Sets a value for the multiplier. Results for the sample are multiplied by this value. Not used by calibration samples.
Divisor	0.000001 to 1,000,000.0 Sets a value for the divisor. Results for the sample are divided by this value. Not used by calibration samples.
Amount Standard	0.000001 to 1,000,000.0 GC Files: Sets the amount of the first internal standard. Used to calibrate results for Internal Standard and Normalized Percent calculations. Not used by calibration samples. MS files: Sets an ISFactor which is used by Analysis and Verification samples. It will be multiplied by the appropriate Compound Calibration Level Amount that is in the DH Method being used. Note that internal standards in Analysis and Verification samples always use the amount that is specified in Calibration Level 1.
MultiChannel MultiStandard	none, multiple, specific channel GC files: Opens the Data Handling Channels dialog box to specify the calibration parameters for up to five different Detector Channels. MS files: Not used by MS data handling. These are GC detector channels which are different from the scan function channels that may be specified in the MS method.
Add	Adds a line to the end of the RecalcList.
Insert	Adds a new line before the highlighted line.
Delete	Deletes the highlighted line in the RecalcList.
Fill Down	Causes the contents of the top cell in a series of highlighted cells to be copied to the cells below it. Used to edit all the cells in a column quickly.

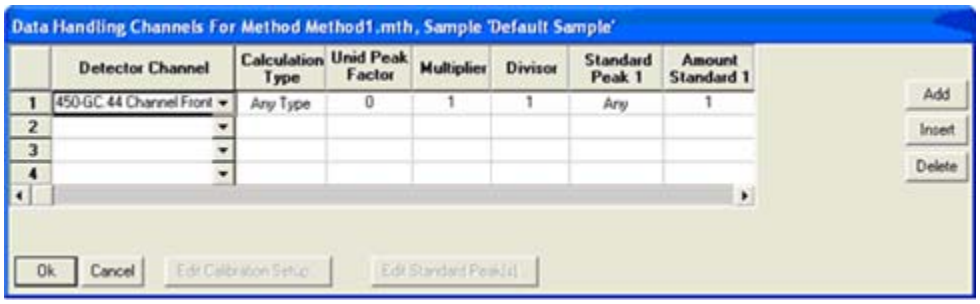
Item	Description
Browse...	Opens the Open Data File dialog box to select a Data File to add to the RecalcList.
Report...	Shows the results report for the selected Data File.
Defaults…	Displays the Set Defaults dialog box, allowing you to specify default values for each applicable field in the RecalcList.
Begin	Opens the Begin RecalcList Dialog Box to specify a method to be used while recalculating or printing all RUN files in this RecalcList, and to then begin recalculating or printing the files.
Suspend	Suspends execution of this RecalcList after the current file has been completed.
Resume	Resumes execution of this RecalcList after it has been suspended.

Data Handling Channels Dialog Box

NOTE: This dialog box is only used to specify standard GC data handling. MS data handling uses only one detector channel.

You can specify the Multiplier, Divisor, and Unidentified Peak Factor on a channel-by-channel basis for up to five different detector channels. And you can specify up to eight internal standards for each of the five channels, for a total of forty internal standards. ***If you only want to specify a single Multiplier, Divisor, Unidentified Peak Factor, and Amount Standard to be used for all channels of all detectors, you may do so directly in the SampleList, RecalcList or Inject Single Sample dialog box and do not need to use this dialog box.***

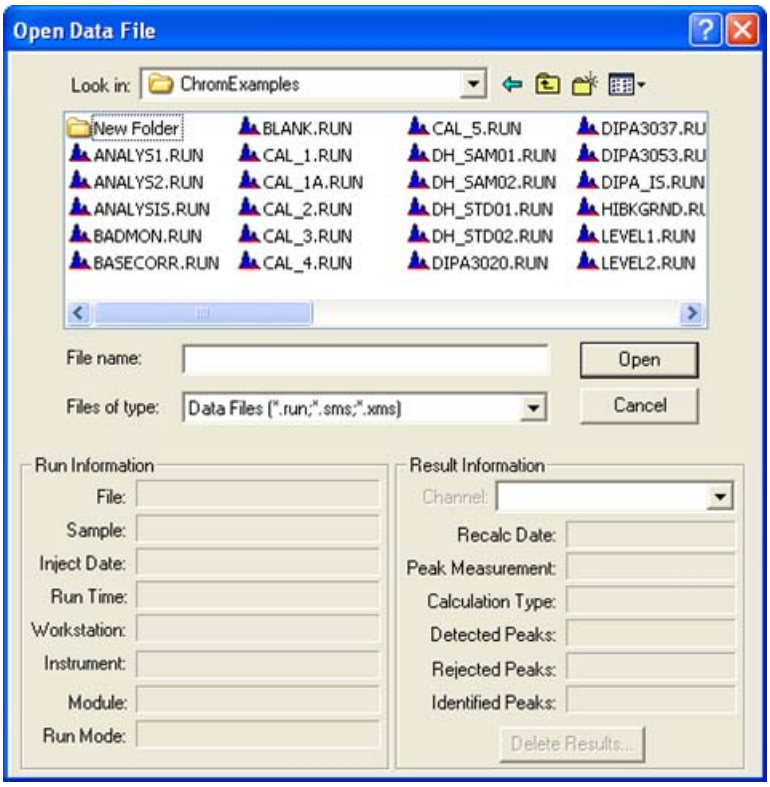
If you plan to specify parameters on a channel-by-channel basis, before opening this dialog box make sure that the active method contains the data handling sections for each channel, and that their peak tables contain the standard peaks (if any) properly named and checked. The dialog box uses information from the active method to help you make the proper specifications for the type of calibration method that you will be using. ***If you later change the standard peak names in the peak table, you will need to revisit this dialog for each sample to update the names and amounts.***



Item	Description
Detector Channel	Indicates the detector channel that is specified by the remaining fields in the row. Channels are indicated by the detector module name, bus address, and channel identifier. The combo box contains entries for all channels having data handling sections in the active method. If the desired channel is not visible in the combo box, make sure that the correct method is active and that it contains data handling sections for the desired channel.
Calculation Type	Internal Std External Std Normalized % No Calibration Indicates the calibration method specified for the detector channel in the active method. To change the calibration method for a specific channel, first click on the channel's row, then click on the "Edit Calibration Setup" push-button. If the Calculation Type is not Internal Std or Normalized %, the "Edit Standard Peak(s)" push-button will be disabled.
Unid Peak Factor	0 to 1,000,000 Sets a calibration factor for unidentified peaks.
Multiplier	0.000001 to 1.000,000 Sets a value for the multiplier. Results for the sample are multiplied by this value.
Divisor	0.000001 to 1,000,000 Sets a value for the divisor. Results for the sample are divided by this value.
Standard Peak 1	40 character standard peak name from peak table Indicates the name of the first Internal Standard Peak. The Amount Standard 1 will be applied to the Internal Standard Peak having the same name. To change the standard peak name for a specific channel, first click on the channel's row, then click on the "Edit Standard Peak(s) push-button.
Amount Standard 1	0.000001 to 1,000,000 Sets the amount of the first internal standard. Used to calibrate results for Internal Standard and Normalized Percent calculations.
Standard Peak 2-8	40 character standard peak name from peak table Indicates names of the multiple internal standard peaks present in the specific channel's peak table. . To change the standard peak names for a specific channel first click on the channel's row, then click on the "Edit Standard Peak(s) push-button. If the peak table does not contain multiple internal standards, these fields will be disabled.

Item	Description
Amount Standard 2-8	0.000001 to 1,000,000 Sets the amounts of the second through eighth internal standards. Used to calibrate results for Internal Standard and Normalized Percent calculations involving multiple internal standards. If the peak table does not contain multiple internal standards, these fields will be disabled.
Add	Adds a line to the end of the list.
Insert	Adds a new row before the highlighted line.
Delete	Deletes the highlighted row in the list.
Edit Calibration Setup	Opens the Calibration Setup Dialog Box to permit inspection and editing of the calibration parameters in the method for the indicated detector channel.
Edit Standard Peak(s)	Opens the Peak Table Dialog Box to permit inspection and editing of the Standard Peak names in the method for the indicated detector channel. Open the Peak Table and press OK to transfer the standard peak names and amounts from the Peak Table to the indicated detector channel row.

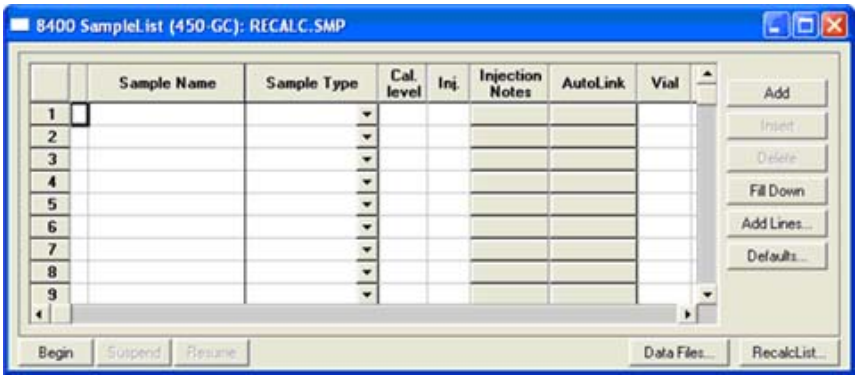
Open Data File Dialog Box



Item	Description
Look in	Lists the available folders and files. To see how the current folder fits in the hierarchy on your computer, click the down arrow. To see what's inside a folder, click it. The box below shows the folders and files in the selected location. You can also double-click a folder or file in that box to open it. To open the folder one level higher, click the “up arrow” button on the toolbar.
File list	Lists the folders and files in the selected location. To see what's inside a folder, double-click it. You can also use the Look In box to see the hierarchy of folders. To open the folder one level higher, click the “up arrow” button on the toolbar.
File name	Shows the currently selected file.
Files of type	Restricts the list of files to only those matching the selected type.
Run Information	Shows information about the currently selected file.
Result Information	Shows information about the results, if any, calculated from the current data file.
Channel	Specifies the detector channel to show Result Information for. Note that this applies only to standard GC results.
Delete Results	Allows you to delete results from the currently select channel of the currently selected data file. This button does not appear if it has been disabled from the Varian MS Workstation Security Administration application. Note that this only affects standard GC results. MS results are not deleted.
Open File	Opens the selected data file using the selected channel.
Cancel	Cancels file selection.

SampleList Window

The SampleList window contains injection parameters that are specific to the sample introduction device you are using on your instrument. This section describes the generic SampleList fields. Refer to the appropriate Instrument Control help topic in the System Control Reference Help for a description of the device-specific extensions to the SampleList.



Item	Description
Sample Name	Up to 19 characters Sets the name of each sample in the SampleList
Sample Type	Baseline, Analysis, Calibration, Verification, Print Calib, New Calib Block, AutoLink, Activate Method Sets the sample type, or automation action, of each line in the SampleList.
Cal. Level	1 to 10 Sets the calibration level of each calibration or verification sample in the SampleList.
Inj	1 to 9 Sets the number of injections to be made of the sample.
Injection Notes	up to 180 characters Opens the Notes window for the selected sample to edit or create a note about the sample.
AutoLink	Two AutoLink commands when Sample Type is Baseline, Analysis, Calibration, or Verification. One AutoLink command when Sample Type is AutoLink. One Activate Method Command when Sample Type is Activate Method. Opens the AutoLink Parameters dialog box to set the options for linking to a remote application during automation through System Control. Opens the Activate Method dialog box to set the path name for activating a new method during automation of a SampleList through System Control.
Unid Peak Factor	0 to 1,000,000.0 Sets a calibration factor for unidentified peaks. Not used by calibration samples.
Multiplier	0.000001 to 1,000,000.0 Sets a value for the multiplier. Results for the sample are multiplied by this value. Not used by calibration samples.
Divisor	0.000001 to 1,000,000.0 Sets a value for the divisor. Results for the sample are divided by this value. Not used by calibration samples.
Amount Standard	0.000001 to 1,000,000.0 GC Files: Sets the amount of the first internal standard. Used to calibrate results for Internal Standard and Normalized Percent calculations. Not used by calibration samples. MS files: Sets an ISFactor which is used by Analysis and Verification samples. It will be multiplied by the appropriate Compound Calibration Level Amount that is in the DH Method being used. Note that internal standards in Analysis and Verification samples always use the amount that is specified in Calibration Level 1.

Item	Description
MultiChannel MultiStandard	none, multiple, specific channel GC files: Opens the Data Handling Channels dialog box to specify the calibration parameters for up to five different Detector Channels. MS files: Not used by MS data handling. These are GC detector channels which are different from the scan function channels that may be specified in the MS method.
Add	Adds a line to the end of the SampleList.
Insert	Adds a new line before the highlighted line.
Delete	Deletes the highlighted line in the SampleList.
Fill Down	Causes the contents of the top cell in a series of highlighted cells to be copied to the cells below it. Used to edit all the cells in a column quickly.
Add Lines…	Displays the Add Lines dialog box, allowing you to specify the number of lines to either insert or append to the spreadsheet, along with the values to use for each applicable field. Certain fields such as Sample ID and vial number can be automatically incremented.
Defaults…	Displays the Set Defaults dialog box, allowing you to specify default values for each applicable field in the SampleList.
Data Files…	Opens the Data File Generation dialog box to specify the naming scheme being used for Data Files generated from injections. Note that if the method contains both MS and standard GC DH method sections, then both sms and run files will be generated.
RecalcList…	Opens the RecalcList Generation dialog box to specify the options for generating or updating RecalcLists after injections. Note that if the method used contains both MS and standard GC DH sections, then the generated Recalc List will contain both sms and run files.

Select SampleList Section Type Dialog Box

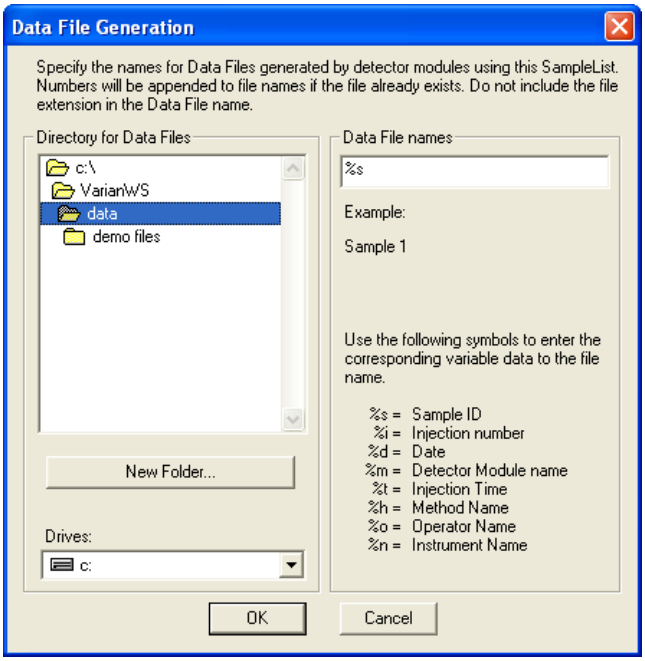
A SampleList File may contain multiple SampleList Sections. Each installed AutoSampler can contribute its own unique type of section, having special features that correspond to its special hardware. For example, the 8200 has syringe sampling mode features, while the 8134 has relay control features. Generally each installed AutoSampler has its own unique SampleList with special columns for its features. A SampleList File can contain a section for each type of AutoSampler, similar to the way that a Method file can contain a section for each type of Instrument Module.

This dialog box lets you pick the specific section that you want to edit in a SampleList file that may contain more than one section.

Item	Description
SampleList section type listbox	Selects a section type to use in building a new SampleList; opens the appropriate SampleList window. SampleLists may contain sections for multiple types of sample handling devices, depending upon which module drivers have been installed.

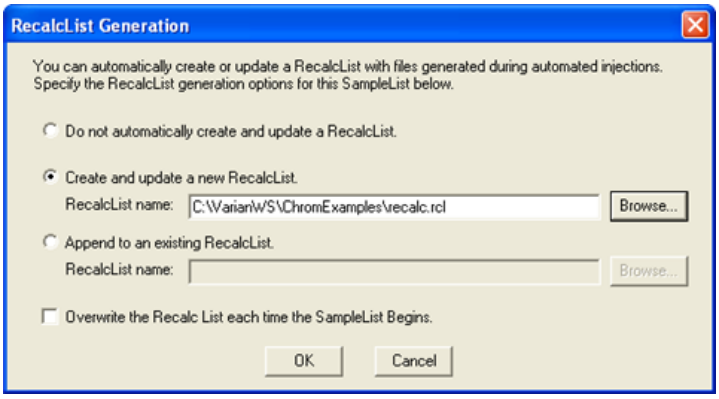
Item	Description
OK	Creates a SampleList section of the specified type.
Cancel	Cancels the SampleList section creation.

Data File Generation Dialog Box



Item	Description
Directory for Data Files	Shows the currently selected directory where Data Files will be generated.
New Folder	Allows you to create and name a new folder in the currently displayed directory.
Drives	Allows you to specify the drive where Data Files will be generated.
Data File Names	Allows you to enter the Data File name specification. You may enter as many characters as you wish, but the final file name (including path) must not exceed 255 characters in length. You may embed the special symbols listed in the window to represent sample-specific information in the Data File name. As you enter the specification, an example file name is displayed.
OK	Accepts the name specification.
Cancel	Cancels the name specification.

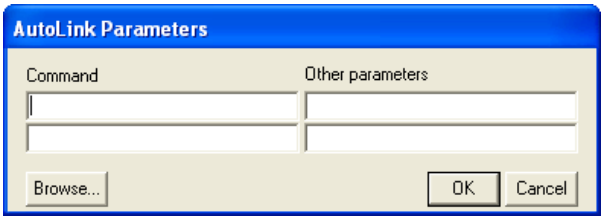
RecalcList Generation Dialog Box



Item	Description
Do not automatically create and update a RecalcList.	No RecalcList will be generated or updated when you create Data Files as a result of injections.
Create and update a new RecalcList	Allows you to enter the name of a new RecalcList that will be created when Data Files are generated as a result of injections. If the RecalcList name that you specify already exists when the injections are performed, a number will be appended to the name so that it is unique.
Append to an existing RecalcList	Allows you to browse for an existing RecalcList file. When Data Files are generated as a result of injections, their information will be appended to this file.
OK	Accepts the RecalcList specification.
Cancel	Cancels the RecalcList specification.

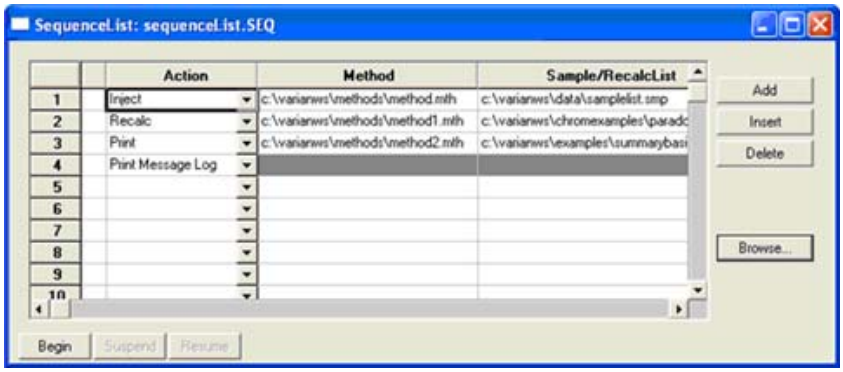
AutoLink Parameters Dialog Box

With AutoLink, you can specify a program to be executed after all injections of a sample have been performed, or two programs to be executed after each injection of that sample. When AutoLink appears as a sample type in a SampleList or RecalcList, the associated program is executed at that point in the SampleList / RecalcList after the previous SampleList / RecalcList line has completely finished. The AutoLink can also be specified as part of a SampleList line that has a Baseline, Analysis, Calibration, or Verification sample type. In such cases, the two AutoLink programs are executed after each injection of the sample.



Item	Description
Command	DOS command lines to open DDE applications Sets the command line that will be used when AutoLink is invoked.
Other Parameters	commands understood by the remote application Provides information to the remote application when it is invoked.
Browse...	Opens the Select an AutoLink Program dialog box to select the name of an AutoLink program and enter it into the Command field.

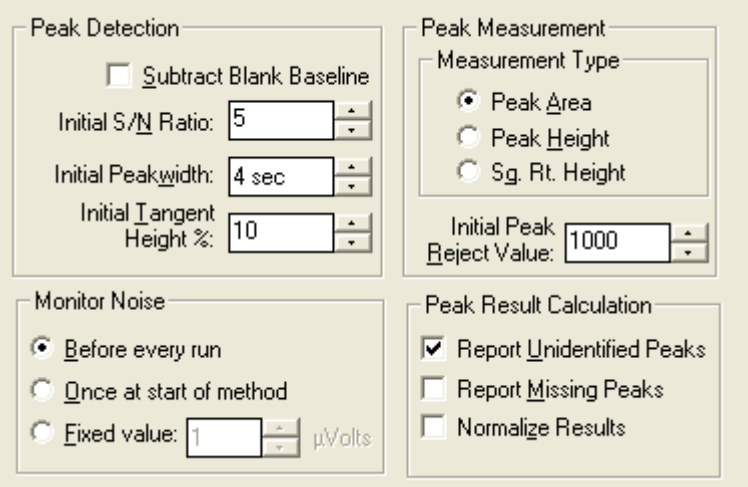
Sequence Window



Item	Description
Action	Shows the action chosen for each line in the Sequence
Method	Shows the Method chosen for each line in the Sequence
Sample/RecalcList	Shows the SampleList or RecalcList chosen for each line in the Sequence
Add	Adds a new line to the end of the Sequence.
Insert	Adds a new line above the highlighted line.
Delete	Deletes the highlighted line in the Sequence.
Browse...	Opens the Select a Method File or Select a Sample/RecalcList window to browse through directories and find a Method or Sample/RecalcList file to add to the Sequence.

GC Data Handling Method Command Reference

Integration Parameters



Peak Detection:

Item	Description
Subtract Blank Baseline	checked or not checked If checked, subtracts the blank baseline in the Method from each Data File. Used to account for predictable changes in the baseline for each run, giving a relatively flat baseline.
Initial S/N Ratio	1 to 256 Sets the initial signal-to-noise ratio for the Method. Used to set the sensitivity of peak detection. This value is overridden if you time program a Signal to Noise Ratio event.
Initial Peakwidth	0.5 to 256 Represents an estimate of the peak width at half height in seconds. Peak detection uses this with the S/N Ratio to discriminate between peaks and noise. It automatically updates the value if you do not program peak width.

Item	Description
Initial Tangent Height %	0 to 100 Sets the percentage of a mother peak's size below which a given peak is considered a tangent peak. Used to assign tangent peak status as a percentage of the mother peak size. Can be used to force a peak to be integrated as a tangent or as a fused peak. This value is overridden if you time program a Tangent Height Percentage event.

Monitor Noise:

Item	Description
Monitor Noise	Before Every Run, Once at Start of Method, Fixed Value Sets times at which the Workstation monitors noise. The workstation can monitor noise before each run, once at the start of each Method, or use a user-specified value between 1 and 10,000 (units depend on detector type).

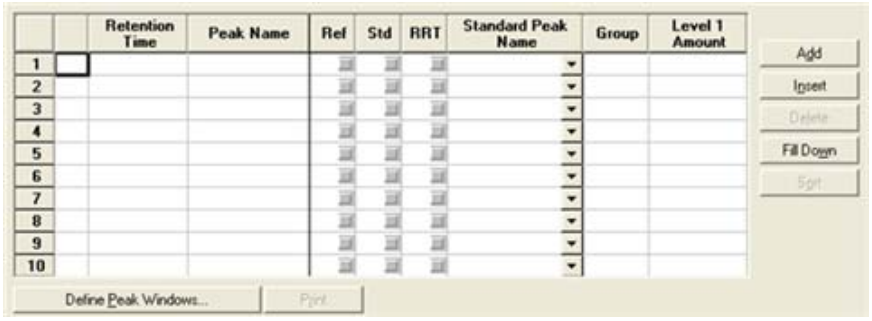
Peak Measurement:

Item	Description
Measurement Type	Area, Height, Square Root of Height Sets the method used to measure the peaks.
Initial Peak Reject Value	0 to 1,000,000 Sets the minimum size peak to be identified. Used to eliminate very small peaks from the report, to ensure that insignificant peaks are not mistaken for peaks of interest. This value is overridden if you time program a Peak Reject value.

Peak Result Calculation:

Item	Description
Report Unidentified Peaks	checked or not checked If checked, tells the Workstation to report all peaks, whether identified or not.
Report Missing Peaks	checked or not checked If checked, tells the Workstation to report any peaks in the peak table that were not found. Used to see which peaks should have been found in the sample but were not.
Normalize Results	checked or not checked If checked, results for each analyte will be expressed as a percentage amount relative to the total amount of all components of the sample. This checkbox is enabled only for external standard and internal standard calculations.

Peak Table

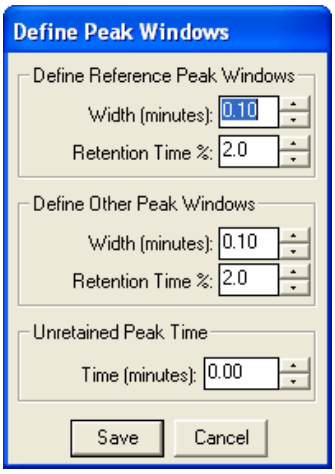


Item	Description
Retention Time	0.001 to 1440.0 Sets the expected retention time of a peak. Specify a retention time at which you expect a peak to elute.
Peak Name	up to 40 characters Assigns a name to a peak. Specify the compound name or some form of identification for the analyte.
Ref	checked or not checked If checked, identifies a peak as a reference peak. Used to account for shifting retention times.
Std	checked or not checked If checked, identifies an internal standard peak. Used to mark which peak represents the internal standard in IS or N% calculations.
RRT	checked or not checked If checked, identifies a peak as a relative retention time peak.
Standard Peak Name	Any standard peak Combobox which allows you to select one of the internal standards to use for this peak.
Amounts (levels 1 to 10)	0.000001 to 1,000,000 Sets the amount of the standard for each level. The number of columns displayed depends on the number of calibration levels specified in the Calibration Setup window.
Add	Adds a peak to the end of the peak table.
Insert	Inserts a peak in the peak table above the active row. Used to insert an entry into the peak table between existing entries.
Delete	Deletes the highlighted peaks from the peak table.
Fill Down	Copies the contents of the top cell in a series of highlighted cells to the cells below it. Used to edit all the cells in a column quickly.
Sort	Reorders the table in order of increasing retention time.

Item	Description
Define Peak Windows...	Opens the Define Peak Windows dialog box to set time windows for reference peaks and other peaks or to set an Unretained Peak Time.
Print	Prints the contents of the current peak table.

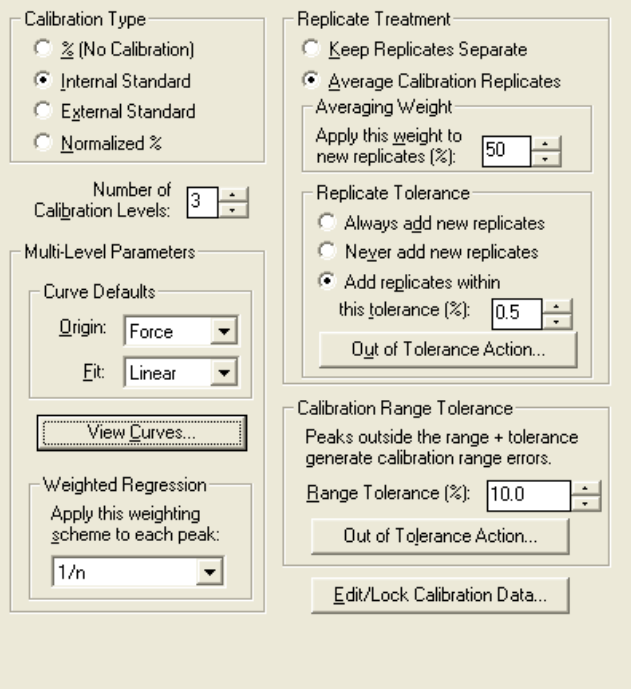
Define Peak Windows Dialog Box

For both types of peaks, you set an absolute time window and a percentage time window. The actual time window used will be equal to the absolute time plus the percentage time.



Item	Description
Define Reference Peak Windows: Width	0.00 to 200.0 Sets an absolute time that will be added to and subtracted from the retention time of a reference peak to define a time window.
Define Reference Peak Windows: Retention Time %	0 to 100 Sets a percentage of the retention time of a reference peak that will be added to and subtracted from the retention time to define a time window.
Define Other Peak Windows: Width	0.00 to 200.0 Sets an absolute time that will be added to and subtracted from the retention time of a non-reference peak to define a time window.
Define Other Peak Windows: Retention Time %	0 to 100 Sets a percentage of the retention time of a non-reference peak that will be added to and subtracted from the retention time to define a time window.
Unretained Peak Time (minutes)	0.00 to 1440.00 Sets the Unretained Peak Time (the amount of time taken by an unretained compound to pass through the chromatograph) for the Method. Used in RRT calculations.

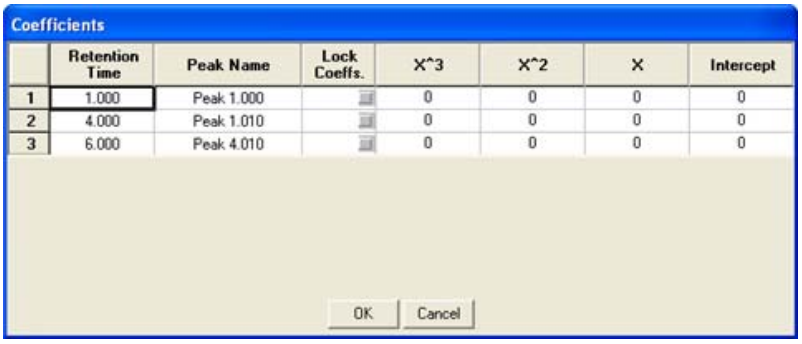
Calibration Setup



Item	Description
Calibration Type	% (No Calibration), Internal Standard (IS), External Standard (ES), Normalized % (N%) Sets the calculation type for the Method. Determines what calculations are performed for calibrations and analyses.
Number of Calibration Levels	1 to 10 levels Sets the number of calibration levels you will be using.
Default Curve Origin	Include, Ignore, Force Sets the default treatment of the origin in each curve. Choose to include, ignore, or force the curves through the origin.
Default Curve Fit	Linear, Quadratic, Cubic Sets the default for how each calibration curve is fit. Choose a linear, quadratic, or cubic equation for the curves.
View Curves...	Opens the Calibration Curve window. Used to view, edit, print, or export the calibration curve.
Weighted Regression	None, 1/n, 1/nX, 1/X2, or 1/nX2 Sets the weighted regression scheme to be used in determining calibration coefficients.

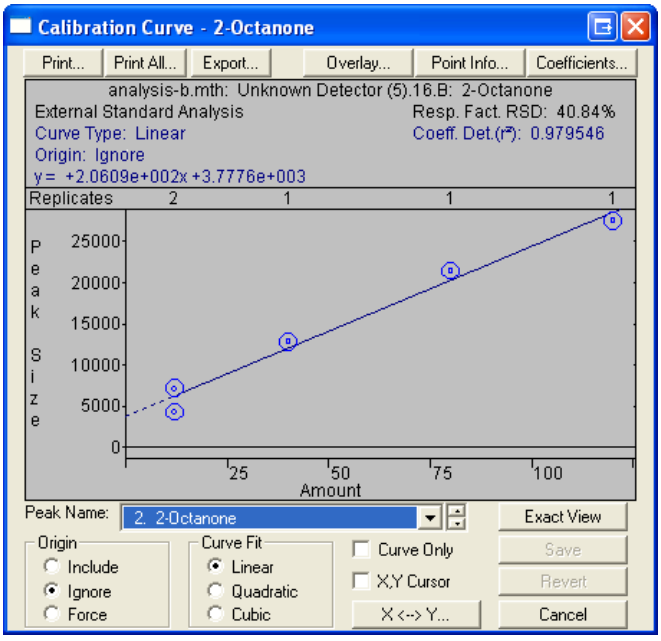
Item	Description
Replicate Treatment	Keep Replicates Separate or Average Calibration Replicates Determines whether new replicates are kept separate or whether they are averaged into an existing historical value. When keeping replicates separate, there is a limit of 10 replicates that can be stored. However, you can indefinitely continue to average new replicates into the historically maintained value.
Averaging Weight	0-100% Sets the weight given to new calibration replicates when averaging into the historical value.
Replicate Tolerance	Always add new replicates, Never add new replicates, Add replicates when within this tolerance (%) Determines whether a new replicate should be added to the calibration curve or whether it should be ignored. Always add new replicates does no verification of replicates -- they are always added. Never add new replicates does not add the replicate and is seldom used. Add replicates when within this tolerance (%) only adds a replicate to the calibration curve if within the tolerance specified. This tolerance is applied the same way as is the Deviation Tolerance for a Verification run.
Replicate Tolerance %	0 to 500% Sets the replicate tolerance value.
Replicate Tolerance Out-of-Tolerance Action	No Action, Increment Error Count, Terminate Sample List, Halt Automation Sets which action is taken when a replicate is of tolerance. Either does nothing (No Action), adds 1 to the error count (Increment Error Count), stops the run and goes to the next SampleList (Terminate Sample List), or halts automation (Halt Automation) each time a replicate is out of tolerance.
Calibration Range Tolerance %	0 to 500% Sets the calibration range tolerance percentage for which peaks outside the calibration range plus the tolerance generate calibration range errors. Zero is always used for the low end of the calibration range check, even if the valid calibration range does not extend to the y axis.
Calibration Range Out-of-Tolerance Action	No Action, Increment Error Count, Terminate Sample List, Halt Automation Sets which action is taken when a replicate is of calibration range. Either does nothing (No Action), adds 1 to the error count (Increment Error Count), stops the run and goes to the next SampleList (Terminate Sample List), or halts automation (Halt Automation) each time a replicate is out of calibration range.
Edit/Lock Calibration Data...	Opens the Coefficients window to edit calibration coefficients for the Method.

Coefficients Table



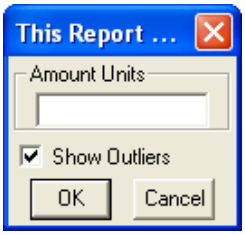
Item	Description
Retention Time	Shows the retention time of each peak.
Peak Name	Shows the name of each peak.
Lock Coeffs.	checked or not checked If checked, coefficients will not be updated on calibration runs. Prevents specific calibration coefficients from changing on subsequent calibration runs. Can be used to manually enter calibration coefficients for peaks that will not be identified in the calibration standard.
coefficients: X^3, X^2, X, intercept	-100,000,000.0 to 1,000,000 Sets the coefficients that define the calibration curve for each peak.

Calibration Curve Window



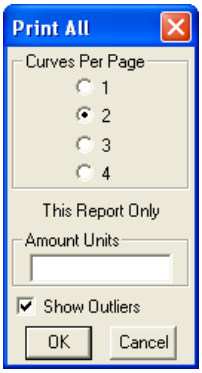
Item	Description
Curve Type	Shows the type of curve fit currently used. Indicates whether the curve fit has been changed since the calibration (edited).
Origin	Shows the origin treatment currently used. Indicates whether the origin treatment has been changed since the calibration (edited).
Equation $y = aX^3 + b X^2 + cX + d$	Shows the equation of the calibration curve currently displayed. Indicates whether the coefficients have been changed since the calibration (edited).
Response Factor RSD	Shows the Relative Standard Deviation of Response Factors.
Corr. Coeff (R^2)	Shows the Correlation Coefficient for the calibration curve.
Print...	Opens the This Report Only dialog box to print only the current calibration curve.
Print All...	Opens the Print All dialog box to print all the calibration curves for the Method.
Export...	Opens the This Report Only dialog box to export the current calibration curve data to another application.
Overlay...	Opens the Overlay dialog box to compare different fits and origin treatments of calibration curves.
Point Info...	Opens the Point Info dialog box to edit outliers from the calibration curve and obtain information about individual points.
Coefficients...	Opens the Coefficients dialog box to edit the coefficients for the calibration curve.
X <--> Y	Opens the X <--> Y dialog box to use the curve to calculate one coordinate from the other.
Revert	Undoes any changes to the curve since it was last saved.
Peak Name	Any peak in the chromatogram Selects a peak for which to view the calibration curve
Origin	Include, Ignore, Force Sets the treatment of the origin in the curve for the current peak. Choose to include the origin, ignore it, or force the curve through the origin.
Curve Fit	Linear, Quadratic, Cubic Sets how the calibration curve for the current peak is fit. Choose a linear, quadratic, or cubic equation for the curve.
Curve Only	checked or not checked When checked, hides the header information at the top of the curve display. Used to enlarge the curve display.
X, Y Cursor	checked or not checked Shows X and Y coordinates on the curve.

This Report Only Dialog Box



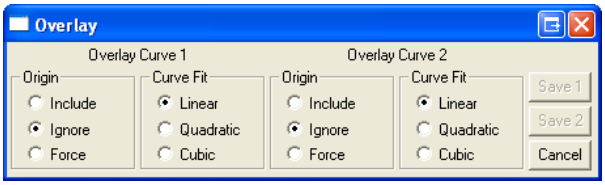
Item	Description
Amount Units	Up to 10 characters Lets you label the units for the amount field of the current calibration curve.
Show Outliers	checked or not checked If checked, outliers appear on the printed calibration curve.

Print All Dialog Box



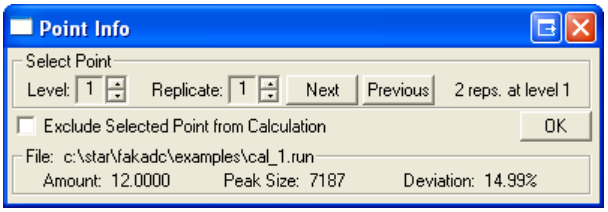
Item	Description
Curves Per Page	1, 2, 3, or 4 Lets you set how many curves will be printed on each page.
Amount Units	Up to 10 characters Lets you label the units for the amount field of the calibration curves.
Show Outliers	checked or not checked If checked, outliers appear on the printed calibration curves.

Overlay Window



Item	Description
Origin	Include, Ignore, Force Sets the treatment of the origin for an alternate curve for the selected peak.
Curve Fit	Linear, Quadratic, Cubic Sets the fit for an alternate curve for the selected peak.
Save 1	Saves overlay curve 1 as the curve for the peak.
Save 2	Saves overlay curve 2 as the curve for the peak.

Point Info Dialog Box

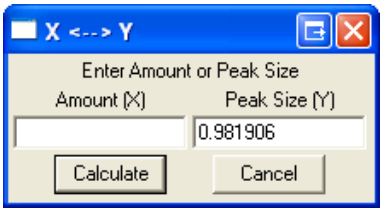


Item	Description
Exclude Selected Point from Calculation	If checked, marks the selected point as an outlier, excluding it from calibration calculations. Excluded points are never lost, and can always be included again at a later time.
Amount	Shows the amount of the standard represented by the selected data point.
Peak Size	Shows the size of the peak represented by the selected data point.
Deviation	Shows, as a percentage, the deviation of the selected data point from the curve. Used to see how far off the selected point is from the result expected from the curve.
Data File	Shows the name of the Data File represented by the selected point.
Level	Specifies the level from which to select a point.
Replicate	Specifies the replicate representing the point. Select a point among those in the selected level.
Next	Select the point at the next highest level on the curve.
Previous	Select the point at the next lowest level on the curve.

Coefficients Dialog Box

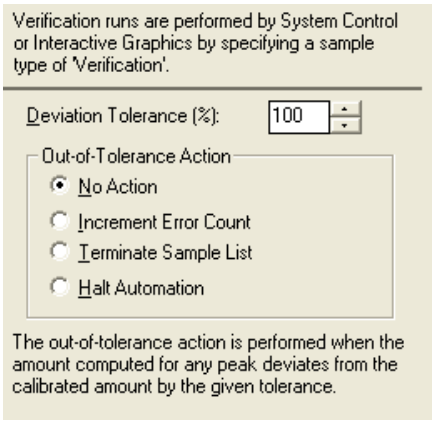
Item	Description
coefficients: X^3, X^2, X, intercept	0.000000 to 1,000,000 Sets the coefficients for each peak.
Restore	Restores coefficients to their last saved values.
Overlay	Shows what the calibration curve would look like with changes to the coefficients by overlaying the new curve on the current curve.
Save	Saves the edited coefficients and closes the Coefficients dialog box.
Cancel	Closes the Coefficients dialog box without saving the edited coefficients.

X <-> Y Dialog Box



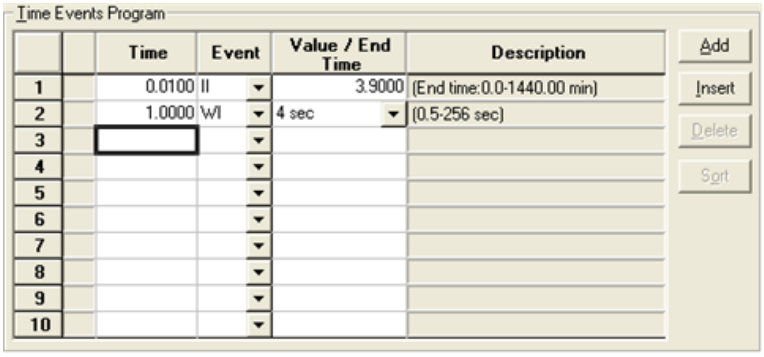
Item	Description
Amount (X) or Amt/Amt Std (X) - depending on calculation type	0.000001 to 99,999,992 Before calculation, shows the amount you enter; after calculation, shows a calculated amount.
Peak Size (Y) or PS/PS Std (Y) - depending on calculation type	0.0 to 99,999,992 Before calculation, shows the peak size you enter; after calculation, shows a calculated peak size.
Calculate	Begins the calculation.

Verification Setup



Item	Description
Deviation Tolerance	0.0 to 500 Sets the percentage of deviation from the calibration curve beyond which a result is considered out of tolerance.
Out-of-Tolerance Action	No Action, Increment Error Count, Terminate Sample List, Halt Automation Sets which action is taken when results for a verification run are out of tolerance. Either does nothing (No Action), adds 1 to the error count (Increment Error Count), stops the run and goes to the next SampleList (Terminate Sample List), or halts automation (Halt Automation) each time a verification fails.

Time Events Table



Item	Description
Start	0 to 1440.0000 Sets the start time for the selected event.

Item	Description
Event	WI, II, GR, VB, SR, FP, SP, HF, HB, HM, SN, TP, and PR. Sets the event type to be added to the table. Choose to add a width (WI), inhibit integrate (II), group (GR), solvent reject (SR), valley baseline (VB) event, forced peak (FP), split peak (SP), horizontal forward (HF), horizontal backward (HB), horizontal minimum (HM), signal to noise ratio (SN), tangent percentage (TP), or peak reject (PR) event.
Value/End Time	Depends on event type For II, GR, SR, VB, FP, HF, HB, and HM events, sets the end time for the selected event. For WI, there are a discrete set of values between .5 and 256 seconds. For SP, the value is not applicable. For SN, the range is 1-256. For TP, the range is 0-100%. For PR, the range is 0-1000000 counts.
Description	Describes the legal values.
Add	Adds the active parameters to the Time Events Table as a new time event.
Insert	Inserts a new row above the highlighted row.
Delete	Deletes the highlighted Time Events Table entry.
Sort	Sorts the table in order of increasing start times.

Time Events

Event	Description
Peak Width (WI)	Changes the data bunching rate to allow for changing peak widths during a run. If no WI events are programmed, Data Handling will automatically adjust the bunch rate as the peak widths increase or decrease. Any time programming of peak widths prevents automatic updating. Used to help reject noise spikes or to prevent gradual baseline changes from being detected as peaks. If a peak is being processed at the programmed time, the event will not occur until a baseline segment is detected. This bunching affects only how Data Handling views the data; it does not have any effect on the raw data bunching set in the Detector Information window for the corresponding detector.
Inhibit Integrate (II)	Suppresses integration of peak area or height. While II is active, peak processing is disabled and no retention times are displayed on the chromatogram or in the results. In addition, any peak being processed at the start of the II event will be aborted. Used to prevent integration over a section of the chromatogram, sometimes to force a baseline to be drawn. II disables peak sensing. In contrast, SR is a post-run filter that rejects detected peaks whose apices fall within the Solvent Reject window.

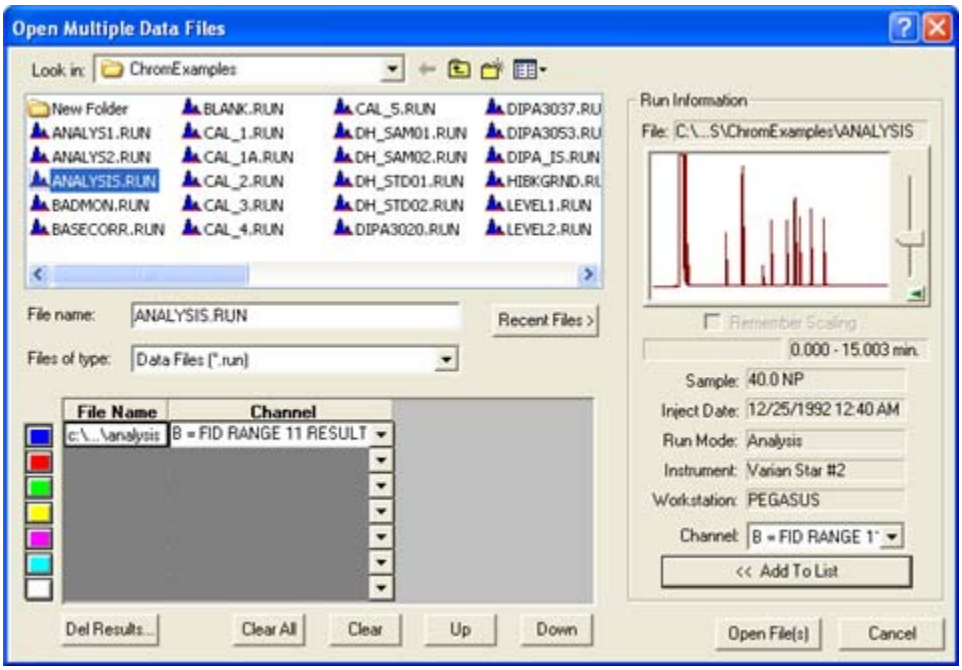
Event	Description
Group Peaks (GR)	Sums the areas of all peaks whose retention times fall within the Group window. This causes all the peaks in this window to be reported as a single peak with the separation code GR and a retention time set to the midpoint of the window. It is a post-integration function. Used to treat all the peaks in a group as if they were a single peak. The Peak Reject filter is applied after the Group function, so that no peaks will be rejected from the Group window because of size. A group peak is treated like any other identified peak.
Solvent Reject (SR)	Rejects all detected peaks whose apices fall within the SR window. It is a post-integration filter. Used to exclude peaks in a certain part of a chromatogram from the report. Unlike the II event, SR can reject a mother peak while retaining its tangent peak in the report.
Valley Baseline (VB)	Forces peak baselines to be drawn through any valley point that occurs during the VB window. It is a post-integration function.
Forced Peak (FP)	Forces integration between the start and end times. A resolved baseline is drawn from the amplitude of the chromatogram at the start time and the amplitude of the chromatogram at the end time. Any Inhibit Integrate events that overlap with a Forced Peak event are ignored. The peak apex is the highest point in the forced peak time range.
Split Peak (SP)	Splits one peak into two peaks. A line is drawn from the chromatogram at the split point to the baseline to separate the original and new peaks. A Split Peak event can be used to split into two peaks a weak shoulder that was not recognized as a separate peak by data handling. If the Split Peak event falls on a baseline section of the chromatogram, the event is ignored.
Horizontal Forward (HF), Horizontal Backward (HB), and Horizontal Minimum (HM)	These events cause a baseline to be drawn horizontally rather than the way it would have been drawn without the event. It does not force a baseline to be drawn, it merely changes the way it is drawn. For Horizontal Forward, the baseline amplitude is at the amplitude of the first peak start event, for Horizontal Backward, the baseline amplitude is at the amplitude of the last peak end event, and for Horizontal Minimum, the baseline amplitude is at the lowest data point in the baseline time range.
Signal to Noise Ratio (SN)	Used to set the sensitivity of peak detection. If a peak is being processed at the programmed time, the event will not occur until a baseline segment is detected. Time programming Signal to Noise Ratio overrides the initial value set in the Integration Parameters Window.
Tangent Percentage (TP)	Sets the percentage of a mother peak's size below which a given peak is considered a tangent peak. Used to assign tangent peak status as a percentage of the mother peak size. Can be used to force a peak to be integrated as a tangent or as a fused peak. Time programming Tangent Percentage overrides the initial value set in the Integration Parameters Window.

Event	Description
Peak Reject (PR).	Sets the minimum size peak to be identified. Used to eliminate very small peaks from the report, to ensure that insignificant peaks are not mistaken for peaks of interest. Time programming Peak Reject overrides the initial value set in the Integration Parameters Window.

GC Interactive Graphics Dialog Boxes

Open Multiple Data Files Dialog Box

NOTE: to quickly open files (when the file list spreadsheet is empty), select them from the explorer style file list and hit the OK button or the return key. You only need to add files to the file list spreadsheet if you want to select a channel different from the default channel.



Item	Description
Look in	Lists the available folders and files. To see how the current folder fits in the hierarchy on your computer, click the down arrow. To see what's inside a folder, click it. The box below shows the folders and files in the selected location. You can also double-click a folder or file in that box to add it to the list of files to open. To open the folder one level higher, click the “up arrow” button on the toolbar.
File list	Lists the folders and files in the selected location. To see what's inside a folder, double-click it. You can also use the Look In box to see the hierarchy of folders. To open the folder one level higher, click the “up arrow” button on the toolbar.
File Name	Selects the file to be added to the list of files to be opened.
Files of Type	Filters the files that you see in the File Name list box so that only Data Files are displayed.
Recent Files	Shows a menu listing up to eight data files that have been recently opened. Selecting one from the menu adds it to the list of files to be opened.
Add To List	Adds the data file specified in the File Name item to the list of files. Up to seven files may be added to the list.
Open Files	Opens the files specified in the spreadsheet. If the spreadsheet is empty, it first adds the files selected in the explorer view to the list. Dismisses the dialog.
Cancel	Closes the dialog and ignores any changes made to the list.

File Name/Channel Table and related commands

The table section of the Open Multiple Data Files Dialog Box is used to assemble the list of files to be opened. You add one or more files to the list by selecting Data File(s) and hitting the Add To List button. Once in the list you can change the color that is associated with the displayed chromatogram by moving the row up or down.

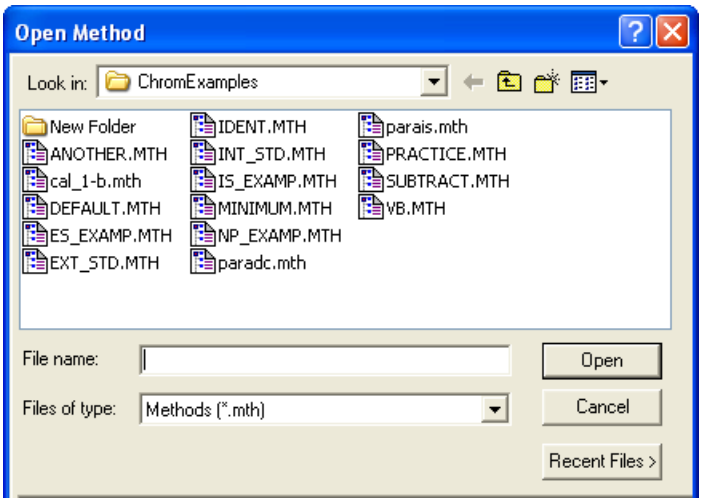
Item	Description
File Name Column	Shows the name of the Data File.
Channel Column	Lets you choose the channel for which to see data. Channels with results have the word "RESULTS" next to the channel label. When a new file is added to the table, the last channel with results is automatically selected.
Delete Results	Deletes the results from the selected channel. Used to remove results from a Data File. The recalculation date and the date of the results deletion will be permanently recorded in the Data File and included in the results report. Enabled by the Security Administration application.
Clear All	Removes all items from the table.
Clear	Removes the selected items from the table. The entire row need not be selected for this button to be enabled.

Item	Description
Up	Moves the selected item up one row. If there is already an entry in the row above, the two entries are exchanged with each other. When moving an item in the top row up, it gets moved to the bottom row.
Down	Moves the selected item down one row. If there is already an entry in the row below, the two entries are exchanged with each other. When moving an item in the bottom row down, it gets moved to the top row.
Colored Buttons	Selects the corresponding row in the table.

Run Information

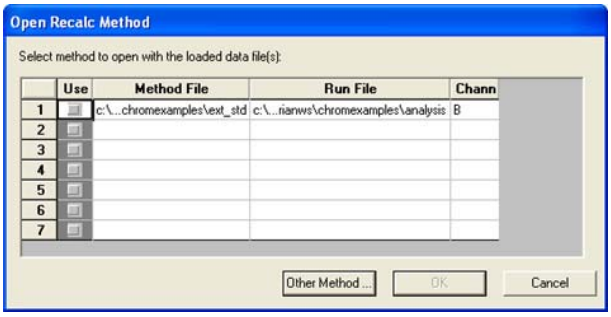
Item	Description
File	Shows the name of the Data File.
Chromatogram Display	Shows a thumbnail view of the chromatogram. This has similar zooming capabilities to the main Interactive Graphics window: click and drag to zoom, click and hold to PowerZoom, double click to zoom to full scale. Note that this autoscales the chromatogram the same way as does the Main Window as described in the Autoscaling section.
Remember Scaling	Check this item to keep the same scaling as you browse through data files. If this item is unchecked, or if the current data file is displayed in full scale, subsequent data files will be displayed in their full scale representation.
Unlabeled field below remember Scaling (left)	Shows the module and address used to collect the data.
Unlabeled field below remember Scaling (right)	Shows the time between run start and run end.
Sample	Shows the name of the sample.
Inject Date	Shows the date of the original run.
Run Mode	Shows the sample type for the selected channel.
Instrument	Shows the instrument used to calculate the current data.
Workstation	Shows the name of the workstation used to collect the data.
Channel	Lets you choose the channel for which to see data. Channels with results have the word "RESULTS" next to the channel label. When a new file is added to the table, the last channel with results is automatically selected.

Open Method File Dialog Box



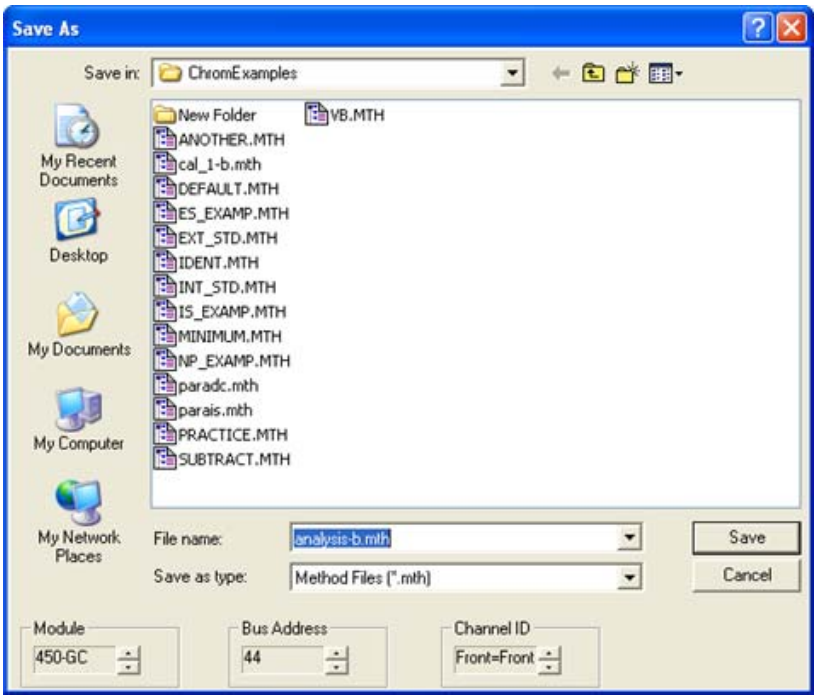
Item	Description
Look in	Lists the available folders and files. To see how the current folder fits in the hierarchy on your computer, click the down arrow. To see what's inside a folder, click it. The box below shows the folders and files in the selected location. You can also double-click a folder or file in that box to open it. To open the folder one level higher, click the “up arrow” button on the toolbar.
File list	Lists the folders and files in the selected location. To see what's inside a folder, double-click it. You can also use the Look In box to see the hierarchy of folders. To open the folder one level higher, click the “up arrow” button on the toolbar.
File name	Shows the currently selected file.
Files of type	Filters the files that you see in the File Name list box so that only method Files are displayed.
Recent Files	Click on this button to display a list of recently selected files. When you select a file from this list, its name is displayed in the File name box.
Open	Opens the selected file.
Cancel	Cancels file selection.

Open Original/Recalc Dialog Boxes



Item	Description
Use	Check this box for the method you wish to open. If you check a box for which the method file listed does not exist, you are asked whether you would like to replace the listed method file with another one.
Method File	The method file you to open.
Run File	The data file from which the method file name was obtained.
Channel	The channel of the data file from which the method file name was obtained.

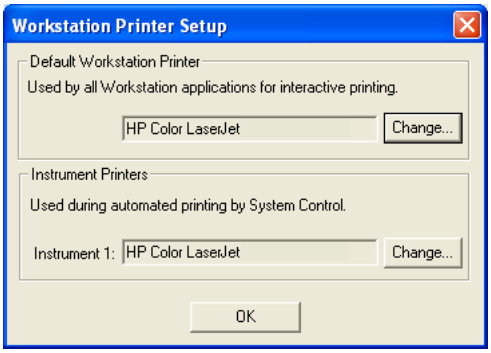
Save Method As Dialog Box



Item	Description
Save in	Specifies the folder into which the method is to be saved. To see how the current folder fits in the hierarchy on your computer, click the down arrow. To see what's inside a folder, click it. The box below shows the folders and files in the selected location. You can also double-click a folder or file in that box to overwrite the Method with that name. To open the folder one level higher, click the “up arrow” button on the toolbar.
File list	Lists the folders and files in the selected location. To see what's inside a folder, double-click it. You can also use the Look In box to see the hierarchy of folders. To open the folder one level higher, click the “up arrow” button on the toolbar.
File name	Enter new file name for the method file to save.
Save as type	Filters the files that you see in the File Name list box so that only method Files are displayed. Also, indicates that files entered without an extension automatically have .mth appended.
Module	Assigns a detector module to the Data Handling section of the Method. Used to change the detector module to which the Data Handling section is assigned.
Bus Address	Assigns a bus address to the Data Handling section of the Method. Used to change the bus address to which the Data Handling section is assigned.
Channel ID	Assigns a channel to the Data Handling section of the Method. Used to change the channel to which the Data Handling section is assigned.

Workstation Printer Setup Dialog Box

This dialog box is used to specify the printers that will be used by Varian MS Workstation applications both interactively and during automation.



Item	Description
Default MS Workstation Printer	Shows the printer used by all Varian MS Workstation applications for interactive printing.

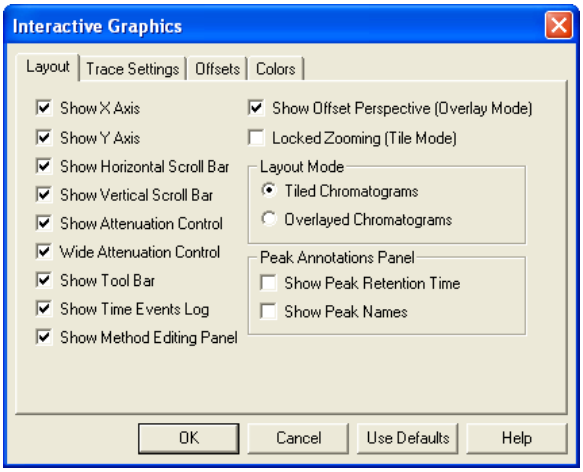
Item	Description
Instrument Printers (Instruments 1-4)	Shows the printers used during automated report printing in System Control (one for each instrument).
Change...	Opens the Print Setup dialog box. Allows you to select a different printer or alter the hardware and software settings for the printer.

Preferences Dialog Box

The Interactive Graphics preferences dialog box is divided into four functional groups in a tabbed dialog. Select the Layout tab to show or hide a particular component of the layout, such as the X axis. Select the Trace Settings tab to affect changes to the Main Window (except for colors), such as whether to show peak names or whether peak events should be drawn as triangles or lines. Use the Offsets tab to control the amount of offset between chromatogram when more than one data file is open and you have selected overlay mode. The Colors tab allows you to configure the window background color and the trace colors.

Whenever you change one of the options listed below, Interactive Graphics automatically redraws the screen to reflect the change you have made. The Use Defaults button sets all of the options to their factory configured settings. Hit the Cancel button if you want to exit the dialog aborting any changes made. The display will be redrawn to reflect the settings in place before you opened the dialog. Use the OK button to exit the dialog and accept any changes you made.

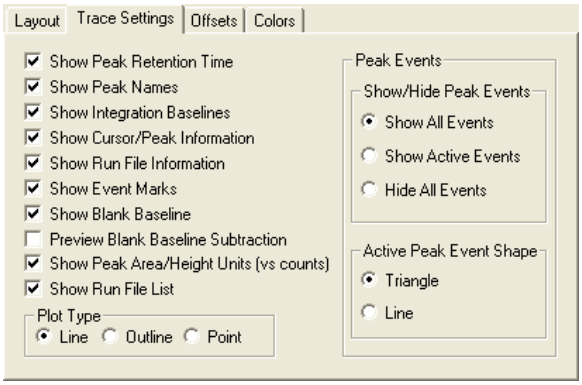
Layout Tab



Item	Description
Show X Axis	Show or hide the time axis.
Show Y Axis	Show or hide the amplitude axis.
Show Horizontal Scroll Bar	Show or hide the horizontal scroll bar.

Item	Description
Show Vertical Scroll Bar	Show or hide the vertical scroll bar.
Show Attenuation Control	Show or hide the attenuation control (to the right of the main window).
Wide Attenuation Control	When displayed, the attenuation control displays a wedge indicating that as you move the slider up, data is zoomed.
Show Tool Bar	Show or hide the chromatogram toolbar.
Show Time Event Log	Show or hide the Time Event Log Panel textual descriptions at the actual times that the Data Handling time events occurred. Holding the mouse over an event marker shows a tool tip with information about one of the thirteen types of Data Handling events: Width (WI), Inhibit Integration (II), Grouped Peak (GR), Valley Baseline (VB), Solvent Reject (SR), Forced Peak (FP) , Split Peak (SP), Horizontal Forwards (HF), Horizontal Backwards (HB), Horizontal Minimum (HM), Signal to Noise Ratio (SN), Tangent Percentage (TP), and Peak Reject (PR).
Show Visual Method Editing Panel	Show or hide the Visual Method Edit Panel (below the x-axis). Use the Visual Method Edit Panel to define a Peak Table and a Time Events Table using visual programming and to visually compare the location of programmed time events versus the actual time the Data Handling time events occurred.
Show Offset Perspective	Displays perspective lines when more than one Data File is open in overlay mode and both the time and amplitude offsets are greater than zero. These perspective lines are a visual aid to help you see the amount of the offset, and for lining up points at the same time on different chromatograms. If the time offset is too great or the amplitude offset too small, the perspective lines are automatically removed.
Locked Zooming (Tile Mode)	Lock Zoom (tiled mode): when depressed, locks the amplitude scaling so that changing the amplitude scaling in one chromatogram causes all other chromatograms to also display the same amplitude range. When not depressed, the amplitude range of the individual chromatograms may differ.
Layout Mode	Tile Chromatograms: displays chromatograms one above each other with each chromatogram in it own non-overlapping section in the main window. In tiled mode, the time axis for all chromatograms is always the same.
	Overlay Chromatograms: displays chromatograms on top of each other so that portions of each chromatogram overlap ones that are visually behind them. In this mode, each trace may be offset from others (as specified in the Offsets tab of the Preferences dialog) to provide a 3-D view of the data.

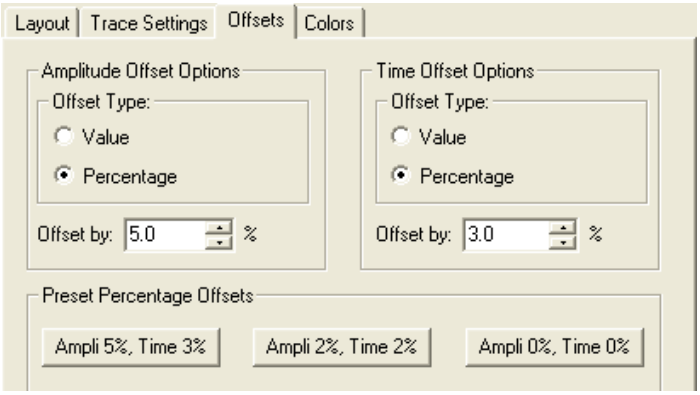
Trace Settings Tab



Item	Description
Show Peak Retention Times	When checked, displays peak retention times in the Main Window for all reported peaks, so even unidentified peak retention times will be displayed.
Show Peak Names	When checked, displays peak names in the Main Window for all reported peaks, so even unidentified peak names will be displayed.
Show Integration Baselines	When checked, displays the peak baselines and lines that drop from valleys to the baseline. If the Data File has never been reintegrated or if results have been deleted, then the Data File doesn't contain baseline information, and this option will have no effect.
Show Cursor/Peak Information	Turns the cursor on or off. The cursor follows the active trace and displays the time and amplitude of it current position in an "info-panel". As you move it near a peak event, it jumps to the peak event and "sticks" to it. If the peak event represents a reported peak apex, then the "info-panel" also displays information such as the peak name, area, and width. Hold the shift key down to disable the "stickiness" feature so that the cursor follows the trace smoothly and is not affected by peak events. Hold the control key down to allow the cursor to move anywhere on the screen without following the active trace.
Show Run File Information	When checked, shows the Run File info-panel which has information about the active data file.
Show Blank Baseline	When checked, displays the blank baseline, if any. Regardless of whether the blank baseline is displayed, the chromatogram trace is offset by the blank baseline data specified by the Preview Blank Baseline Subtraction (below).

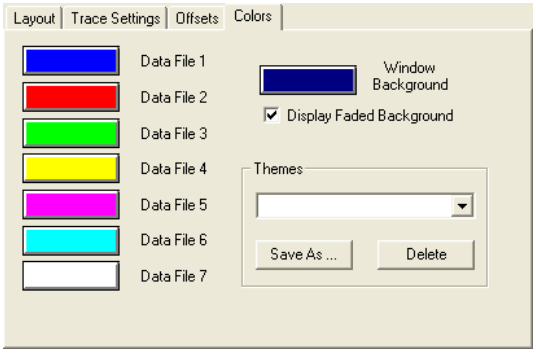
Item	Description
Preview Blank Baseline Subtraction	When checked, uses the blank baseline data from the active Method. When unchecked (the default), uses the blank baseline data from the data file as it was used for the most recent recalculation. The blank baseline data is used both for blank baseline display and to offset the chromatogram trace (see above). In many cases, there may be no blank baseline data present in either the method or the data file, in which case no blank baseline is displayed and the chromatogram trace is not adjusted. When checked and there is blank baseline data in the method, this lets you visualize the effect of subtracting a particular blank baseline from a chromatogram trace without first needing to recalculate with the blank baseline. Also, in this mode you can modify individual blank baseline points.
Plot Type	Line Plot: plots chromatograms as a continuous line.
	Outline Plot: plots chromatograms as a continuous line and individual points are outlined with a rectangle.
	Point Plot: plots chromatograms as a series of points. In point plots, each point represents a single data point in the raw Data File. Zooming the display in point or outline mode lets you see individual data points.
	NOTE: all data points may not be drawn when zoomed to full or large scale. That is because the data is reduced at large scales so that only important data is displayed. This is especially apparent when the data has been oversampled. Also, when the trace goes off the screen, additional points may be drawn at the edge of the window that are not actual data points, but represent an interpolated point between the point in the window and the next one just outside of the window.
Show/Hide Peak Events	Show All Events: all traces have peak events drawn. Peak events for the active chromatogram may be drawn as a line or triangle (see Active Peak Event Shape below). The non-active chromatograms always have their peak events displayed as a line.
	Show Active Events: only the active trace has peak events drawn as a line or triangle (see Active Peak Event Shape below).
	Hide All Events: no traces have any peak events displayed.
Active Peak Event Shape	Displays the peak events for the active chromatogram as either a line or a triangle. You can only move peak events for the active trace, and only when its peak event shape is a triangle.

Offsets Tab



Item	Description
Offset type:	Determines whether the number in the Offset by field is an absolute value or a percentage of the screen height or width.
Offset by	If more than one chromatogram is open, enter the amount of vertical or horizontal spacing between chromatograms. The offset has no effect when only one chromatogram is open. Note that when entering an offset by amplitude or time value, the offset at one zoom level may be too large or small at another zoom level.
Preset Percentage Offsets	These buttons allow you to quickly change between a few preset values. These switch the offset type to Percentage and automatically enter the values indicated in the Offset by field.

Colors Tab

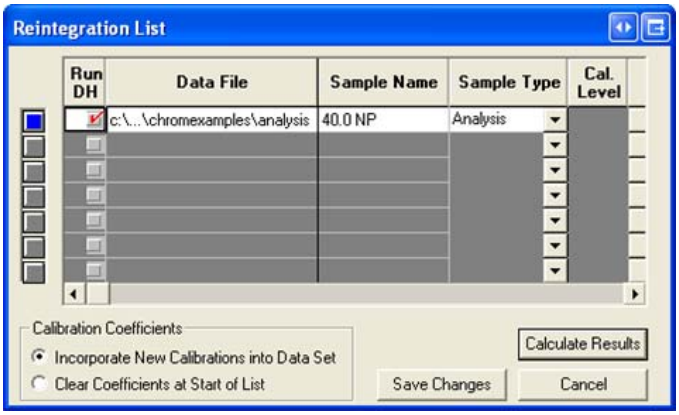


Item	Description
Data File 1 – 7	These buttons indicate the colors of the seven data files you can open in Interactive Graphics. Click on a button to bring up the standard Windows Color dialog for selecting a color for the trace.

Item	Description
Window Background	Select the color for the Main Window background. Click on a button to bring up the standard Windows Color dialog so that you can select a new background color for the window. With a dark background color, Interactive Graphics automatically chooses white as the color for axes, info-panels, etc. text. With a light background color, the text color is automatically set to black.
Display Faded Background	When checked, the selected color fades to a lighter color from the bottom to the top of the window. When solid black or white is selected, the fading does not occur.
Themes combo-box	Select from one of the color themes to change all of the color settings at once.
Save As …	Saves the current color selection. This opens a dialog box into which you enter the name of the theme to save. This saves the colors for the seven data files, the window background color, and whether the background color is faded.
Delete	Deletes the current theme.

Reintegration List Dialog Box

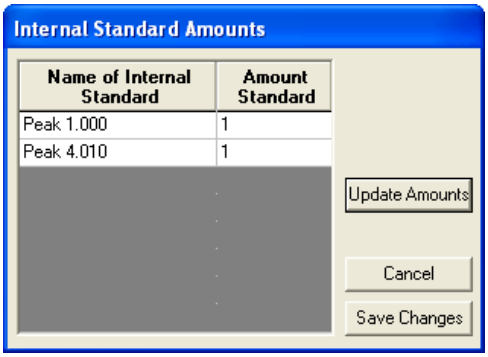
NOTE: Post-run reporting actions specified in the active Method (such as ASCII File Conversion) are not done when you perform a recalculation from Interactive Graphics.



Item	Description
Colored buttons	Selects the corresponding active row in the table.
Run DH	Marks which files will be recalculated. Files without a check mark will not be recalculated.
File	Shows the name of the Data File

Item	Description
Sample Name	Up to 19 characters Shows the sample name for a Data File. This field may not be edited.
Sample Type	Blank Baseline, Analysis, Calibration, Verification Sets the sample type for a Data File, to establish how each Data File should be treated during recalculation.
Cal. Level	1-10 Sets the calibration level of a calibration or verification Data File.
Internal Standard	Button which opens the Internal Standard Amounts Dialog Box to set the amounts of one or more internal standards. Used to calculate results for internal standard and normalized percent calculations.
Unidentified Peak Factor	0.00001 to 999999 Sets a calibration factor for unidentified peaks. Used to calculate results for unidentified peaks.
Multiplier	0.00001 to 999999 Sets a value for the multiplier. Results for the sample are multiplied by the value.
Divisor	0.00001 to 999999 Sets a value for the divisor. Results for the sample are divided by the value.
Recalc Notes	Button which opens the Recalc Notes Dialog. Notes entered in this dialog can be displayed by the Report application by selecting the Notes option in the Results Format portion of the Report section of the Method.
Incorporate New Calibrations into Data Set/ Clear Coefficients at Start of List	If Incorporate New Calibrations is chosen, keeps existing coefficients and adds new data to them. If Clear Coefficients is chosen, zeroes all coefficients in the Method
Save Changes	Save changes made and dismiss the dialog.
Calculate Results	Saves changes made and starts the recalculation.

Internal Standard Amounts Dialog Box



Item	Description
Name of Internal Standard	Lists the names of the internal standards. You can get a copy of this list from the peak table using the Update List button (see below), but you may not edit these. Use the Peak Table Dialog Box to edit these names.
Amount Standard	Edit these values to change the amount of internal standard.
Update List *or* Update Amounts	Copies the current list of internal standards and their amounts from the peak table to the table described above. After copying the list, the button changes to Update Amounts. This allows you to recopy just the amounts from the Peak Table after modifying them.
Cancel	Dismisses the dialog box without saving any changes.
Save Changes	Dismisses the dialog box and saves any changes made.

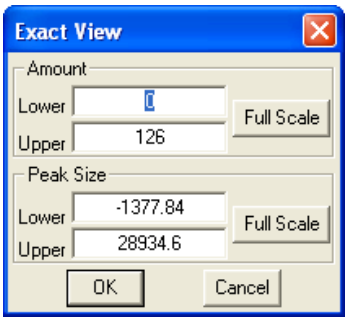
Fill Peak Table Window

The Fill Peak Table option opens a smaller version of the Peak Table window. It allows you to fill the table quickly with the peaks in the active chromatogram. In this mode the cursor is automatically displayed and locks on to the nearest peak apex. Clicking adds a new peak table entry. If you check the “Fill table from selection” checkbox in the Fill Peak Table Window, then all of the peaks in the region you select are added to the peak table. After peaks have been added to the table, you can either edit their parameters in this window or in the full Peak Table window.

Item	Description
Retention Time	0.001 to 1440.0 Displays the retention time of the peak that was clicked on.
Peak Name	up to 40 characters Assigns a name to a peak.
Ref	If checked, identifies a peak as a reference peak.
Std	If checked, identifies an internal standard peak in IS or N% calculations.

Item	Description
RRT	If checked, identifies a relative retention time peak.
Standard Peak Name	List of all peaks marked as an internal standard Allows selection of the peak that will be used as the internal standard for this peak.
Group	Any integer Allows you to assign an arbitrary group number to a peak. A report can be generated organized by number.
Amounts (levels 1 to 10)	1e-6 to 1,000,000 Sets the amount of the standard for each of the calibration mixtures, level by level.
Add	Adds a peak to the peak table as a new entry.
Insert	Inserts peak in the peak table above the active row.
Delete	Deletes the highlighted peaks from the peak table.
Sort	Sorts the rows by retention time.
Fill table from selection	Sets the mode so that all of the peaks in the region you select are added to the peak table as opposed to just the individual peak on which you click.

Exact View Dialog Box



Item	Description
Start Time (Minutes)	Sets the time at which the plot will start.
End Time (Minutes)	Sets the time at which the plot will end.
Low Amplitude	Sets the lowest amplitude that will appear on the plot. Enter this in the units as currently displayed by the y-axis.
High Amplitude	Sets the highest amplitude that will appear on the plot. Enter this in the units as currently displayed by the y-axis.

GC Interactive Graphics Menus

File Menu

Menu Item	Description
Add/Remove Chromatogram …	Opens the Open Multiple Data Files dialog box to select a list of up to seven data files and view their chromatograms; all currently open chromatograms are replaced with chromatograms selected in the dialog.
New Method	Opens a new Untitled Method to edit; closes any previously open Method.
Open Method	Opens the Open Method dialog box to open an existing Method file to edit; closes any previously open Method.
Open Original Method	Opens the Open Original Method dialog box to open for editing the Method used with the original injection; closes any previously open Method.
Open Recalc Method	Opens the Open Recalc Method dialog box to open for editing the Method used with the most recent recalculation; closes any previously open Method.
Build Method from Datafile …	Extracts the data handling method used for the most recent recalculation which is stored in the data file. You will be prompted to save the method file with the default name 'DatafileName-Channel.mth'. Closes any previously open Method.
Save Method …	Saves the Method with all changes to Data Handling sections.Use this Method for runs or recalculations.
Save Method As …	Opens the Save Method As … dialog box to save a Method under a new name.
Print …	Prints the Main Window as viewed on the screen except that the background is drawn white. When printing to a monochrome printer, any colors on the screen are drawn black instead. Opens the standard Windows print dialog allowing you to select the printer and number of copies to print. When the dialog is first opened, the Default MS Workstation Printer is selected.
Print Method	Prints the Data Handling section of the Method.
Print Preview …	Opens the Print Preview Window, and displays the Chromatogram as it will be printed. There may be minor layout differences between the main window display and the printed output, Colors are modified as described in the Print menu item. From the Print Preview Window, you can print the window and zoom in to examine details.
Print Setup …	Opens the MS Workstation Printer Setup dialog box to set preferences for printing.
Exit	Closes Interactive Graphics.

Edit Menu

Menu Item	Description
Undo	Undo is not available.
Cut	Cut is not available.
Copy	Copies the main window as a Picture (Windows enhanced metafile format) to the clipboard. This Picture can be resized and the contents will stretch to fit the new frame. This copies a picture with a white background. Any white traces are drawn black; other colors are preserved.
Copy Bitmap	Copies a Bitmap to the clipboard. The bitmap is the size of the main window and cannot be resized. In addition to the main window, this also includes the chromatogram toolbar, the attenuation control, and the Visual Method Edit Window if these are displayed. This copies the screen exactly as drawn without changing background or trace colors.
Copy Picture to Disk	The same as Copy (above) except that it copies a Picture (placeable enhanced metafile format) to a disk file, rather than to the clipboard.
Paste	Paste is not available.
Delete	Deletes any time events or peak events selected in the Visual Method Edit Window.

View Menu

Menu Item	Description
Locator Window	Shows or hides the locator window. This window displays a full scale version of the active chromatogram. When you select a region in this window, it zooms the main window instead. The active chromatogram is either the top most trace in overlay mode, or the bottom most trace in tile mode.
Method Quick Link Button	Shows or hides the Method Quick Link Toolbar containing the Method Quick Link Button. The Method Quick Link button lets you view or print the method file currently open in Interactive Graphics.
Main Toolbar	Shows or hides the main application tool bar, which contains buttons such as the Add/Remove Chromatogram button, the Print button, and the reintegration buttons.
Status Bar	Shows or hides the Status bar at the bottom of the Interactive Graphics window.
Visual Method Edit Window	Shows or hides the a window beneath the x-axis that you use to interactively edit the peak table and the time events table.

Menu Item	Description
Chromatogram Toolbar	Shows or hides the tool bar associated with the chromatogram, which contains buttons such as the Full Scale Button, the Cursor Display Button, and the Tile and Overlay Buttons.
Attenuation Control	Shows or hides the Attenuation Control to the right of the main window. This allows you to scale the amplitude of the displayed trace(s).
Preferences …	Displays the Preferences dialog box to configure settings for how chromatograms are displayed in Interactive Graphics.

Results Menu

Menu Item	Description
Reintegration List …	Opens the Reintegration List dialog box to recalculate results for one or more Data Files. This lets you enter sample related information: whether to run data handling at all for a data file; whether it's an analysis, calibration, baseline, or verification run; recalc notes; etc.
Reintegrate Now	Uses the settings in the Reintegration List to perform a recalculation on the open chromatograms. Used to recalculate results for one or more Data Files without opening the Reintegration List dialog box.
Reintegrate Now/Clear Moved Events	Same as Reintegrate Now, except that any user defined peak start and end points are reset before reintegrating.
Autosave method before Reintegration	When checked, any changes to the method are saved before reintegrating without prompting. When unchecked, you are prompted whether to save any changes to the method before reintegrating. If the method is a memory based method (like a new Untitled method), then you are always prompted to save the method regardless of the setting.
View Calibration Curves …	Opens the Curve Manager window to view calibration curves for the current Method.
Data File Name/Channel	Displays the Quick Link menu for each open Data File. This is equivalent to Data File Operations Quick Link Button on the MS Workstation Toolbar.

Edit Method Menu

Menu Item	Description
Set Password …	Opens the Add Password Dialog Box which allows you to add or change the password for a method file.
Method Notes …	Opens the Method Notes window to edit notes for the Method
Integration Parameters …	Opens the Integration Parameters Dialog Box to edit the integration parameters for a Method.
Peak Table …	Opens the Peak Table Dialog Box to edit the peak table for a Method.
Time Events …	Opens the Time Events Table Dialog Box to edit the time events for a Method.
Calibration Setup …	Opens the Calibration Setup Dialog Box to specify calibration parameters.
Verification Setup …	Opens the Verification Setup Dialog Box to specify verification parameters.
Fill Peak Table …	Opens the Fill Peak Table window to fill the peak table quickly.
Add Method Item	Contains a submenu which allows you to add a Peak Table Entry or one of the 13 Time Events to the Visual Method Edit Window. A better way to add Peak Table Entry or a Time Event is to click with the right mouse button in an empty section of the window. This will bring up the same menu, with the advantage that the event is placed at the location of the right mouse click.
Select All Method Items	Selects all the Peak Table Entries and Time Events in the Visual Method Edit Window.
Delete Selected Method Items	Deletes all selected Peak Table Entries and Time Events in the Visual Method Edit Window.

Help Menu

Menu Item	Description
Help Topics	Displays the help you are now viewing.
Product Support Web Site	If you have Internet access and a web browser installed on your computer, this option will automatically open the Varian MS Workstation Product Support Web Site. Here you will find the latest software and documentation updates for the Varian MS Workstation suite of products, along with additional notes, tips, and answers to frequently asked questions.
About Interactive Graphics	Displays the About Box for the Interactive Graphics application. The About Box contains information about the software version, installation information, and a list of the instrument control modules that you have installed.

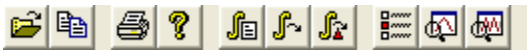
GC Interactive Graphics Toolbars

Toolbar Overview

There are two toolbars on the main window: the Main Toolbar and the Method QuickLink Toolbar. These can each be dragged with the left mouse button to a docked or undocked location. The third toolbar is the Chromatogram Toolbar. It may not be dragged or undocked, however, it can be scrolled out of view by clicking on the green “minimizer” button.

Each toolbar can be hidden or closed. If the toolbar is hidden, it may be displayed by selecting the appropriate menu item from the View menu of Interactive Graphics.

Main Toolbar



	Opens the Open Multiple Data Files dialog box to select a list of up to seven data files and view their chromatograms; all currently open chromatograms are replaced with chromatograms selected in the dialog.
	Copies the main window as a Picture (Windows enhanced metafile format) to the clipboard. This Picture can be resized and the contents will stretch to fit the new frame. This copies picture with a white background. Any white traces are drawn black; the other colors are preserved.
	Prints the Main Window as viewed on the screen except that the background is drawn white. When printing to a monochrome printer, any colors on the screen are drawn black instead. Opens the standard Windows print dialog allowing you to select the printer and number of copies to print. When the dialog is first opened, the Default MS Workstation Printer is selected.
	Displays the help you are now viewing.
	Reintegration List: opens the Reintegration List dialog box to recalculate results for one or more Data Files. This lets you enter sample related information: whether to run data handling at all for a data file; whether it’s an analysis, calibration, baseline, or verification run; recalc notes; etc.
	Reintegrate Now: uses the settings in the Reintegration List to perform a recalculation on the open chromatograms. Used to recalculate results for one or more Data Files without opening the Reintegration List dialog box.

	Reintegrate Now/Clear Moved Events: same as Reintegrate Now, except user defined peak start and end points are reset before reintegrating.
	View Preferences: displays the Preferences dialog box to configure settings for how chromatograms are displayed in Interactive Graphics.
	Toggle Locator Window: shows or hides the locator window. This window displays a full scale version of the active chromatogram. When you select a region in this window, it zooms the main window instead. The active chromatogram is either the top most trace in overlay mode, or the bottom most trace in tile mode.
	Toggle Monitor Window: shows or hides the monitor window. Shows the noise segment acquired before every run. You can change how the noise is monitored using the data acquisition section of the module method (typically specifying the data rate and the monitor length). You can change how the noise is used for peak detection in the Integration Parameters section of the Data Handling method.

Method Quick Link Toolbar

	This button lets you view or print the method file currently open in Interactive Graphics.

Chromatogram Toolbar

	Shows or hides the toolbar.
	Full Scale: zooms all traces to their full scale values. This button is the same as double clicking in the main window.
	Vertical Full Scale: in overlay mode zooms the amplitude range so all traces are visible in the given time range. In tile mode the active (bottom) chromatogram is zoomed so all of the trace is visible in the time range. If zooming is locked, then other chromatograms are zoomed to the same vertical scaling as the active chromatogram. If zooming is not locked, then only the bottom chromatogram is affected. This command only affects the displayed amplitude range, the time range is unaffected. This button is the same as double clicking in the Y axis of the main window.
	Horizontal Full Scale: in overlay mode, zooms such that the entire time range is visible for all chromatograms. In tile mode, the active (bottom) chromatogram is zoomed such that the entire time range is visible. The other chromatograms are zoomed to the same time range as the active chromatogram. This command only affects the displayed time range, the amplitude range is unaffected. This button is the same as double clicking in the X axis of the main window.

	Previous Scaling: zooms to the previous time and amplitude range. Interactive Graphics adds the new scaling rectangle to the end of a list. Previous scaling zooms to the value stored in the previous position. This is disabled at the start of the list.
	Next Scaling: zooms to the next time and amplitude range. Interactive Graphics adds the new scaling rectangle to the end of a list. Next scaling zooms the display to the value stored in the next position on the list. Since new scaling rectangles are added to the end of the list. Next Scaling is available when you had hit the Previous Scaling button. That is, this item is disabled at the end of the list.
	Exact View: opens the Exact View dialog , specify the time and amplitude ranges numerically.
	Cursor Display: turns the cursor on or off. The cursor follows the active trace and displays the time and amplitude of it current position in an “info-panel”. Near a peak event, it jumps to the peak event and “sticks” to it. If the peak event is a peak apex, then the “info-panel” displays information. Hold the shift key down to disable the “stickiness” feature so that the cursor follows the trace smoothly and is not affected by peak events. Hold the control key down to allow the cursor to move anywhere on the screen without following the active trace.
	Select Background Color: opens the standard Windows Color dialog so that you can select a new background color for the window. With a dark background color, Interactive Graphics automatically chooses white as the color for axes, info-panel, etc. text. With a light background color, the text color is automatically set to black. Select “Display Faded Background” so that the selected color fades to a lighter color from the bottom to the top of the window. When solid black or white is selected, the fading does not occur.
	Tile Chromatograms: displays chromatograms one above each other with each chromatogram in its own non-overlapping section in the main window. In tiled mode, the time axis for all chromatograms is always the same.
	Overlay Chromatograms: displays chromatograms on top of each other so that portions of each chromatogram overlap ones that are visually behind them. In this mode, each trace may be offset from others (as specified in the offsets tab of the preferences dialog) to provide a 3-D view of the data.
	Lock Zoom (tiled mode): when depressed, locks the amplitude scaling so that changing the amplitude scaling in one chromatogram causes all other chromatograms to also display the same amplitude range. When not depressed, the amplitude range of the individual chromatograms may differ.
	Fill Peak Mode: opens the Fill Peak Table Window which allows you to quickly build a peak table using peaks from the current chromatogram. In this mode the cursor is automatically displayed and locks on to the nearest peak apex. Clicking adds a new peak table entry. If you check the “Fill table from selection” checkbox in the Fill Peak Table Window, then all of the peaks in the region you select are added to the peak table.
	Calculate Noise for Displayed Data: calculates the noise for the currently displayed section of the chromatogram. To select a time range, zoom a specific area in the interactive chromatogram. See “Using GC Interactive Graphics” on page 187 for more information.

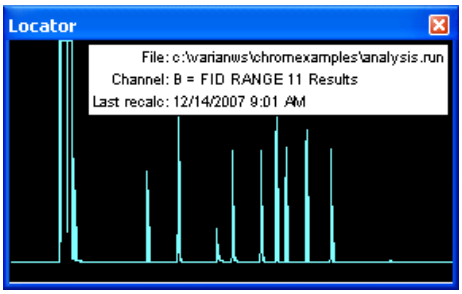
GC Interactive Graphics Window

Locator Window

Use the Locator Window to view the entire active chromatogram and to select a section of the chromatogram to view in greater detail in the Main Interactive Graphics Window. The active chromatogram is either the top most chromatogram in overlay mode, or the bottom most trace in tile mode.

The Locator Window is a window that floats above the main Interactive Graphics window. Interactive Graphics draws a full scale version of the active chromatogram in this window. As implied by the name, you can use this window to quickly locate and zoom to a particular part of the chromatogram by dragging the mouse to create a rectangular selection. This section of the chromatogram is then expanded to fill the entire Main Window. Selecting a section in the Locator Window to view may be faster than scrolling in the Main Window. The section of the chromatogram displayed in the Main Window is indicated by an inverted background in the Locator Window.

An “info-panel” display lists the currently displayed data file name in the Locator Window along with the channel and last recalc data.

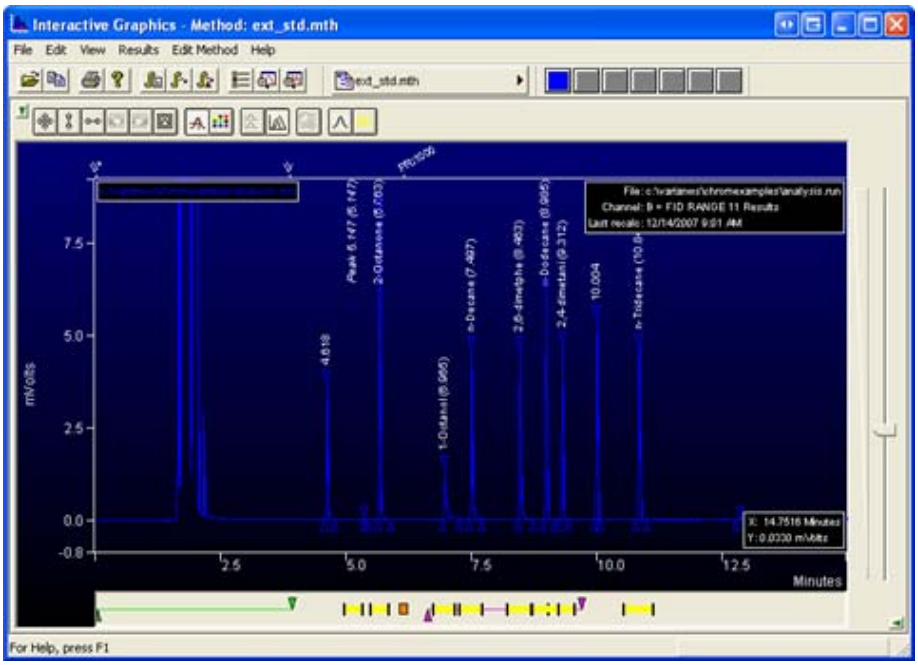


The following mouse actions are possible for the Locator Window:

Action	Effect of Action
Left mouse button click and drag a selection.	Expands selected section of chromatogram to fill the entire Main Window.
Left mouse button double click.	Expands the Main Window to display the entire active chromatogram

Main Window

Use the Main Window to view and manipulate between one and seven chromatograms. This is the main window you use when working with Interactive Graphics.



The Main Window occupies the center of the Interactive Graphics window. The following other panels may optionally be displayed around the periphery of the Main Window:

Panel	Location Relative to Main Window	Purpose
Amplitude Axis Panel	To Left	Y-axis display, vertical zooming
Time Axis Panel	Below	X-axis display, horizontal zooming
Visual Method Edit Panel	Below Time Axis	Interactive peak table entry and time event table editing.
Time Events Log Panel	Above	Display log of time events and the time that they actually occurred.
Chromatogram Toolbar Panel	Above Time Events Log	Quick access to often used functions.
Attenuation Control Panel	To Right	Adjust amplitude range using logarithmic scaling.

Active Chromatogram

When in overlay mode, the Main Window always displays one active chromatogram, and may also show up to six more inactive chromatograms. The active chromatogram is the front-most chromatogram and is the only chromatogram for which you can:

1. Modify the baseline by moving a peak start/end event to a new location.

2. Show a cursor and its associated “info-panel” containing the time and amplitude of the cursor and peak information.

3. Display baselines and droplines.

4. Display peak names and retention times.

5. Show the Time Events that were performed by data handling.

6. Display a blank baseline.

7. Display peak events in the shape of a triangle.

8. Display the run file “info-panel”.

9. Use the scaling buttons from the Chromatogram Toolbar: Full Scale, Vertical Full Scale, Horizontal Full Scale, Previous Scaling, Next Scaling, and Exact View.

You can make an inactive chromatogram the active one, by clicking directly on the chromatogram in the Main Window with the right mouse button and select the Move to Front menu item from the menu displayed.

When in tile mode, all chromatograms are considered active, however, the Chromatogram Toolbar buttons only apply to the chromatogram at the bottom.

Opening Data Files

Use the Open Multiple Data Files dialog box to provide a list of which Data Files will be displayed in the Main Window. You can also use this dialog box to change the order of already open chromatogram(s) which also has the affect of displaying the trace in a different color.

Zooming and Scrolling

The primary purpose of the Main Window is to allow you to inspect sections of the chromatogram and review the placement of peak events as determined by data handling. To do this you may want view a part of the chromatogram in high detail. You do this by zooming, that is, selecting a rectangular section of the chromatogram by dragging the mouse in the Main Window. When you release the mouse, the chromatogram is redrawn so that the selected area fills the entire Main Window. You can zoom similarly by selecting a chromatogram section in the Locator Window. By repeatedly selecting rectangles in the Main Window, you view the chromatogram ever finer detail. Interactive Graphics will not allow further zooming if the amplitude range would become less than 0.0001 and the time range would become less than 0.05 minutes. Double clicking in the Main Window displays the chromatograms at their full scale zoom levels.

“PowerZooming” is an alternative way of zooming. You PowerZoom by clicking and holding the left mouse button down without moving it. This zooms in on that point isometrically, or, if your are holding the control key down, zooms out from

that point. Once PowerZooming begins, you can move the mouse around while the mouse button is still down to change the point at which you are zooming.

You can view other sections of the chromatogram while maintaining the same zoom level by scrolling. Scroll bars are displayed only if the time or amplitude range of your zoomed view is less than the maximum time or amplitude range of the chromatograms as determined by autoscaling. Scrolling horizontally lets you see sections of the chromatogram earlier or later than the current section. Scrolling vertically lets you see sections of higher or lower amplitude.

You can scale vertically using the Attenuation Control to the right of the Main Window. This adjusts the amplitude range on a logarithmic scale. When using the attenuation control, the lowest point of the active trace is fixed, and the amplitude range is adjusted to a smaller range as you slide the position indicator up and to a larger range as you slide it down.

You can zoom in the amplitude and time axes in the same way as you do in the Main Window. You can select a rectangular section of the axis, PowerZoom, and double click in the axis. These actions zoom just like they would in the Main Window, except that only the amplitude scaling is affected when zooming in the amplitude axis and only the time scaling is affected when zooming in the time axis.

Autoscaling

Interactive Graphics automatically determines the maximum and minimum values in the chromatogram. In determining these values, it ignores any chromatogram sections during which an Inhibit Integrate (II) or a Solvent Reject (SR) time event is in effect. It uses these values when displaying a chromatogram at full scale. So when you double click in the Locator Window to expand the Main Window to display the entire active chromatogram, the chromatogram is displayed so that the minimum and maximum amplitudes are at the bottom and top of the window.

Moving Baselines

You can modify baselines and droplines by clicking on a peak start/end event for the active chromatogram and dragging it to a new location. Notice that as you drag a peak event, the Main Window Information Panel will display the type of event being moved, and will constantly update the time and amplitude of the new peak event location. You must reintegrate to view the effects of the moved peak events on the results. Peak information for affected peaks will not be available once a peak event is moved.

NOTE: You can only modify baselines when the peak event shape is a triangle. Moving baseline points is disabled when the peak event shape is a line, or when peak events are not displayed.

All events can be moved other than peak apices or events generated by the use of a Forced Peak (FP) and Split Peak (SP) time events. An easy visual way to determine if a peak event can be moved is to slowly move the mouse over a peak event. If the peak event can be moved, the mouse cursor will change from the cross cursor to the arrow cursor, otherwise, the cursor looks like:  In either case, a tool tip window is displayed showing the time, amplitude, and type of peak event.

A peak event can be moved to within one tenth of one data point in time of an adjacent peak event. By default, a peak event can only be moved so that it touches the chromatogram trace. Hold the control key down while dragging the peak event to move it away from the chromatogram trace. Peak events are drawn as solid triangles or thick lines when moved as opposed to hollow triangles or thin lines when in the original position determined by data handling.

To reset a peak event to the original position determined by data handling, click on the event with the right mouse button and select the Reset to Original Position menu item displayed. To reset all moved peak events to their original position, select Reintegrate Now/Clear Moved Events from the Results menu.

When a peak event has been moved manually, peaks whose areas are affected by the moved event are marked in the report with a ‘U‘, designating a user defined endpoint.

Viewing Options and Mouse Operations

You can customize the appearance of the Main Window with many options that you can set using the View Menu Commands and the Preferences dialog box.

The following mouse actions are possible for the Main Window:

Action	Effect of Action
Left mouse button click and drag a selection.	Expands selected section of chromatogram to fill the entire Main Window.
Left mouse button double click.	Zooms to full scale.
Left mouse click and hold	Zooms isometrically from the mouse position
Left mouse button click on a peak event and drag to a new location.	Moves the peak event to a new location to change the position of baselines and droplines. You must reintegrate to view the affects of the moved event on the results.
Right mouse click on a chromatogram trace.	Brings up a context sensitive menu with actions to be taken for the selected chromatogram. The menu will vary depending on your installation. However, Remove, Move to Front, and Show Run File Info are always present.
Right mouse click on a peak event.	Brings up a context sensitive menu with the action to be taken for the selected peak event. Select the menu choice to reset a moved peak event to its original position.

Info-Panels

Info-panels are rectangular panels that are drawn in the Main Window. There are several of these panels containing information. Some, like the peak counter in Fill table from selection mode, appear only while a particular operation is taking

place. Others, like the run file info-panel, are displayed or hidden depending on a preference setting.

When you move the mouse over an info-panel, the hand cursor is displayed indicating that the info-panel can be moved by dragging it to a new location. Info-panels retain their position relative to the nearest corner of the Main Window, so that when the Interactive Graphics window is temporarily sized to be small and then the size is restored, the original info-panel position is retained.

You can configure the information displayed in an info-panel by right clicking on the info-panel and checking or unchecking items from the menu that is presented.

Neither the position of an info-panel, nor the configured list of items are retained when the data file is closed and then reopened. These are reset to default values when the data file is reopened.

Cursor Info-Panel

When the cursor display is enabled, the cursor info-panel is automatically also displayed. The contents of this info-panel varies depending on the location of the cursor. Usually, it displays only the time and amplitude of the cursor location. When the cursor is at a peak apex, the info-panel also shows peak apex information, such as the name and its area (see below). When moving a peak event it shows the peak event type as well as the time and amplitude of the peak event position. The peak event info-panel is automatically displayed while you are dragging a peak event even when the cursor display is disabled.

NOTE: to show the cursor, select the View>Preferences menu item, then select the Trace Settings Tab and check the Show Cursor/Peak Information checkbox. Alternatively, click on the Cursor Display button on the Chromatogram Toolbar.

Item	Description
Time	The time of the cursor location.
Amplitude	The amplitude of the cursor location.
Name	The name of the peak.
Result or Rsp. Ratio	The calculated results for the peak. For a calibrated peak, this will show the response ratio instead of the results.
Area, Height, or Sq. Root Height	The area, height, or square root of height for the peak, depending on the Peak Measurement type selected in the Integration Parameters Data Handling Method section.
Width	The peak width at half height in seconds.
Type	The type of peak event being moved.

Run File Info-Panel

The Run File info-panel shows information about the active data file.

NOTE: to show the Run File information, select the View>Preferences menu item, then select the Trace Settings Tab and check the Show Run File Information checkbox.Or, right-click a chromatogram trace and select Show Run File Info. Regardless of which chromatogram trace you click, only the run file information for the active trace is displayed.

Item	Description
File	The full path name of the active chromatogram.
Channel	To displayed channel of the active chromatogram.
Last recalc	The date and time the file was last reintegrated.

Fill Peak Table Info-Panel

This info-panel displays the time range of the selection and the count of peaks when filling a peak table from a selection.

NOTE: to show the Fill Peak Table Info-Panel, select the Fill Peak Table item from the Edit Method menu, then and check the Fill table from selection checkbox. Alternatively, click on the Fill Peak Mode button on the Chromatogram Toolbar and check the Fill table from selection checkbox.

Item	Description
Start time	The start time of the selected region.
End time	The end time of the selected region.
Num peaks	The number of peaks that are in the selected region and that will be added to the peak table when the mouse is released.

Visual Method Edit Window

Use the Visual Method Edit Window to define a Peak Table and a Time Events Table using visual programming and to visually compare the location of programmed time events versus the actual time the Data Handling time events occurred.

To use the Visual Method Edit Window, make the window visible by selecting Visual Method Edit Window from the View menu. Or, select Show Visual Method Editing Panel from the Layout tab of the Preferences dialog. Then you can add, remove, move the position, and edit peak table entries and time events using left and right mouse actions. Although most of these actions are also available from the Edit Method menu, once you are familiar with them, you will find the mouse actions a much faster and more direct way of editing time events.

Types of Peak Table Entries

There are four different types of peak table entries. They are all drawn as a solid bar with handles at each end. Click and drag in the middle of the bar to adjust the time of the peak table entry. Click and drag on a handle at either end to adjust the peak window retention time percentage for all peaks. The color of the peak table entry indicates its type. Note that an entry may have more than one color:

Color	Type of Peak Table Entry
Blue	Reference peak
Red	Standard peak
Green	Relative retention time peak
Yellow	None of the above – a normal peak

Types of Time Events

There are two types of time events possible. How they are defined, how they are drawn, and the actions you can take depend on whether it is a time range event or a value event:

Type of Time Event	How Defined	Events of this type (color)	How Displayed
Time range time event.	Start time and end time.	II (green) GR (yellow) VB (purple) SR (dark blue) FP (red) HF (light brown) HB (brown) HM (black)	Up triangle at start time, down triangle at end time, and connecting line all drawn in color of the event.
Value time event.	Value -- units depend on type of event, for instance, area counts for the Peak Reject event.	WI (light blue) SP (olive) SN (dark green) TP (dark purple) PR (orange)	Rectangle in color of the event.

Adding New Peak Table Entries and Time Events

You add a new peak table entry or time event by right clicking an empty spot (i.e. not on an existing time event) in the Visual Method Edit Window and selecting from the displayed menu listing all time events and the peak table entry. The item is added to the window at the location which you clicked. Alternatively, you can add a new time event by selecting from the Add Method Item submenu in the Edit Method menu. If the item is a range time event, the time range is given a default value of one twentieth of the currently displayed time range. If the item is a value time event, the Time Events Table dialog box is displayed with the newly added line selected. This presents an opportunity to set the value of the event. No dialog is presented for the Split Peak value time event since there is no value associated with this event.

Editing Peak Table Entries and Time Events

You can later change any aspect of any time event or peak table entry by double clicking on an item in the Visual Method Edit Window. If you double click on a peak table entry, the Peak Table dialog box is displayed with the row containing that peak event selected. If you double click on a time event, the Time Events Table dialog box is displayed with the row containing that time event selected. You can change any time or value in these dialog boxes, and when you dismiss the dialog, any changes will be reflected in the Visual Method Edit Window.

Selecting Peak Table Entries and Time Events

You select a peak table entry or time event by clicking on it with the left mouse button. If you click on another peak table entry or time event, any selected ones are deselected before the one you clicked on is selected. If you are holding the shift key while clicking on peak table entries or time events, all items you click on will become selected. If you are holding the Control key down while clicking on peak table entries or time events, the selection state of the item is toggled. That is, selected items are deselected, and unselected items are selected.

You can also select a range of peak table entries and time events by clicking with the left mouse button on an empty spot in the Visual Method Edit Window and dragging the mouse cursor. Any items that intersect the displayed rectangle are selected when you release the mouse. As with single clicks, holding the shift key down while selecting a range of peak table entries or time events selects any previously unselected items. Holding the control key down while selecting a range of items toggles the selection state of any item; any previously selected items are deselected while any previously unselected items are selected.

Moving Peak Table Entries and Time Events

You move time events by clicking on them and dragging them to a new location. If you click on the left or right handle of a peak table entry, then you adjust the peak window retention time percentage for all peaks. If you click on the triangle section of a range time event, then you move only the start or end time of the event, the other end stays at the same time. Note that if you move the end time before the start time or vice versa, when you let go of the mouse, the ends will automatically be switched to the right order. If you click on the connecting line section of a peak table entry or range time event, or if you click on a value time event, or if more than one event is selected, then when you drag the mouse, you move the item(s) to a new time. The ability to move multiple time events while maintaining the same time spacing is an easy yet powerful way of making global changes to the method. In particular with peak table entries, this is the easiest way to interactively adjust for retention time drift.

Deleting Peak Table Entries and Time Events

Delete peak table entries and time events by selecting them and hitting the Delete key, using the Delete Selected Method Items from the Edit Method menu, or hitting the Control-D key combination.

Info Window and Mouse Cursor Types

Moving the mouse and pausing over a time event in the Visual Method Edit Window brings up a window containing information about the peak table entry or time event in a condensed format. The window is automatically hidden as soon as you move the mouse.

Notice that as you move your mouse in the Visual Method Edit Window, the mouse will change from a cross cursor to the arrow cursor when over a time event. The arrow cursor indicates you can do one of the several actions with the left or right mouse. If you click with the left mouse on a range time event triangle, notice that the cursor changes to a double-pointed cursor with arrows pointing left and right. This indicates you can move the start or end time for this event.

Right Mouse Menus

Clicking on a peak table entry or time event with the right mouse button displays a context sensitive menu of actions you can do with that item. If only one peak table entry or time event lies underneath the mouse you can edit or delete the item. If there are multiple peak table entries or time events at the same location as where you clicked the mouse, all of these items are listed in the menu, each with Move to Front, Edit, and Delete menu items. If there are multiple selected items, then the menu will contain a list of all the selected items rather than the items at the location you clicked. For peak table entries and time events that lie underneath the front most time event, the Move to Front menu item deselects all other items, selects the indicated peak table entry or time event, and moves if to the front enabling you to more easily manipulate that item.

As described in Adding New Peak Table Entries and Time Events, clicking with the right mouse button in an empty section of the Visual Method Edit Window displays a menu allowing you to add a new peak table entry or time event to the window.

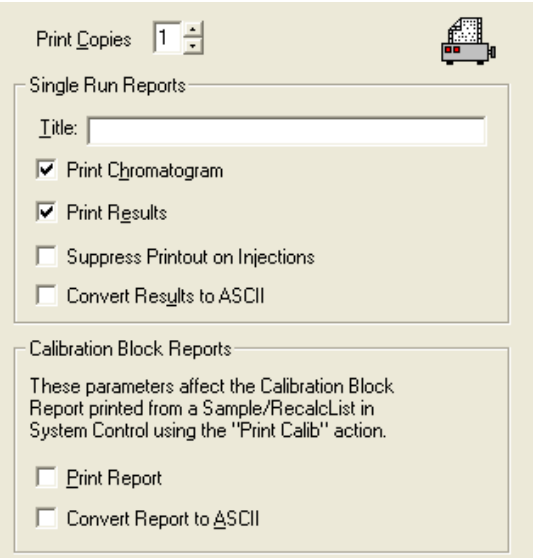
The following mouse actions are possible for the Main Window:

Action	Effect of Action
Hold mouse still over a peak table entry or time event	Displays a window containing information about the item in a condensed format.
Left mouse button click on a peak table entry or time event.	Selects items as described in the Selecting Peak Table Entries and Time Events section.
Left mouse button click in an empty section.	Deselects all peak table entries and time events.
Left mouse button click on a peak table entry or time event and drag.	Moves or sizes items as described in the Moving Peak Table Entries and Time Events section.
Left mouse button click in an empty section and drag.	Selects items as described in the Selecting Peak Table Entries and Time Events section.
Left mouse button double click on a peak table entry or time event.	Displays the Peak Table or Time Events Table dialog box with the row containing the item selected.

Action	Effect of Action
Right mouse button click on a peak table entry or time event.	Brings up a context sensitive menu with actions to be taken for one or more items. Select from the list of Move to Front, Delete, or Edit menu items as described in Right Mouse Menus above.
Right mouse button click in an empty section.	Brings up a context sensitive menu allowing you to add a new peak table entry or time event as described in Adding New Peak Table Entries and Time Events.

GC Standard Report Method Command Reference

Print Options



Single Run Reports:

Item	Description
Title	Up to 60 characters Assigns a title to the report.
Print Chromatogram	When checked, the Workstation prints the chromatogram from System Control during automation.
Print Results	When checked, the Workstation prints the results report from System Control during automation.
Suppress Printout on Injections	When checked, only prints automated reports for Recalc and Print Sequence actions. Used to insure that printer errors do not interrupt an automated sequence of injections
Convert Results to ASCII	When checked, the Workstation converts the results to ASCII. Used to generate results for use in other ASCII-compatible programs.

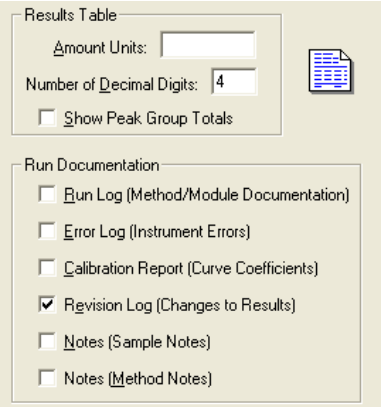
Calibration Block Reports:

Item	Description
Print Report	Selects whether or not a Calibration Block Report is printed when a Print Calib sample type is used in a SampleList or RecalcList (from System Control/Automation).
Convert Report to ASCII	When checked, converts the calibration block report to ASCII format when a *Print Calib* sample type is used in a SampleList or RecalcList (from System Control/Automation).

Other Commands:

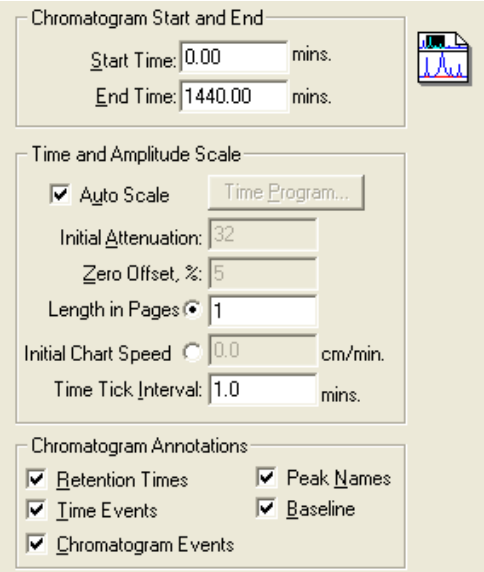
Item	Description
Print Copies	1 to 9 Sets the number of copies of the report to be printed.

Results Format



Item	Description
Units	Any units, up to 10 characters Assigns a name for the units used in the results report.
Number of Decimal Digits	0 to 6 Sets the number of digits in which results are to be expressed.
Run Log	If checked, includes the method and the Time Events Log at the end of the report. Entries in the Time Events Log correspond to the actual times when the events occurred.
Error Log	Includes error messages that occurred during the run at the end of the report. Error messages generated by post-run Data Handling are always printed whether the error log option is active or not.
Calibration Report	Includes the text of the calibration block report as part of the results report.
Notes	Includes notes you entered when you made the injection (original notes) and when you recalculated (appended notes) as part of the report.

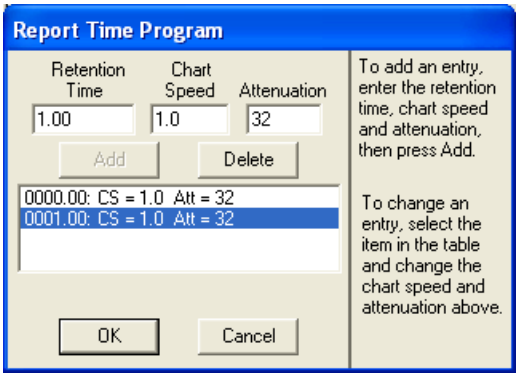
Chromatogram Format



Item	Description
Start Retention Time, mins	0.00 to 1440.00 Specifies a start time after injection for the chromatogram display and printout.
End Retention Time, mins	0.01 to 1440.00 Specifies an end time for the chromatogram display and printout. If the End Retention Time is greater than the actual end time in the data file, the actual end time is used.
Initial Attenuation	1 to 4096 Sets the initial scaling of the display or printout. Attenuation is relative to the maximum full scale value of the detector. An attenuation of 1 scales the chromatogram so that a signal 1/4096th of the detector's full scale is the largest signal that will be printed. The attenuation can be changed to other values at various times by time programming. The initial attenuation value is ignored if you select Auto Scale.
Zero Offset, %	-100 to 100 Sets the zero point of the displayed or printed chromatogram as a percentage of the full page. Larger values let you record negatively drifting baselines or negative chromatographic peaks. The zero offset value is ignored if you use Auto Scale.
Length in Pages	0 to 9 Sets the number of pages used to print a chromatogram. This option takes precedence over the chart speed value. The chart speed is calculated by dividing the total length in pages by the run time.

Item	Description
Initial Chart Speed, cm/min	0.0 to 30.0 Sets the initial chart speed for the printout. This speed does not change unless you time program the chart speed. Set the Length in Pages to 0 to use this option.
Minutes per Tick	0.0 to 10.0 Sets the interval between time tick marks on the printout.
Auto Scale	If checked, adjusts the attenuation and zero offset so that the chromatogram fills the screen or page.
Time Events	If checked, annotates the right margin of the chromatogram to show when time events occurred. Shows when peak width (WI), inhibit integrate (II), solvent reject (SR), group (GR), valley baseline (VB), chart speed (CS), and attenuation (ATT) changes occurred.
Chromatogram Events	If checked, annotates the chromatogram with tick marks that denote peak event for peak starts, peak ends, apices, and valley points.
Retention Times	If checked, annotates the chromatogram with the retention times for all detected peaks.
Peak Names	If checked, displays peak names for identified peaks.
Baseline	Draws baseline segment lines under the peaks.
Edit Time Program...	Opens the Report Time Program dialog box to edit a report time program.

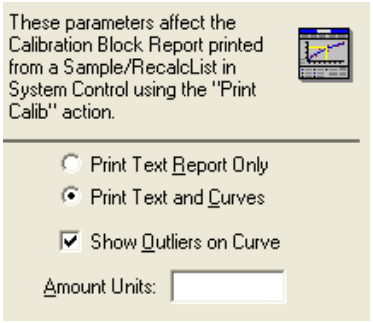
Report Time Program Dialog Box



Item	Description
Retention Time	0.00 to 1440.0 Sets the start time for the selected event.
Chart Speed	0 .1 to 30.0 Sets the program chart speed.
Attenuation	1 to 4096 Sets the program attenuation.. Attenuation is relative to the maximum full scale value of the detector. An attenuation of 1 scales the chromatogram so that a signal 1/4096th of the detector's full scale is the largest signal that will be printed.

Item	Description
Add	Adds the active parameters to the program list. To add a change in chart speed or attenuation to the report time program.
Delete	Deletes the highlighted line in the program. To delete a line in the report time program, canceling that change in chart speed or attenuation.

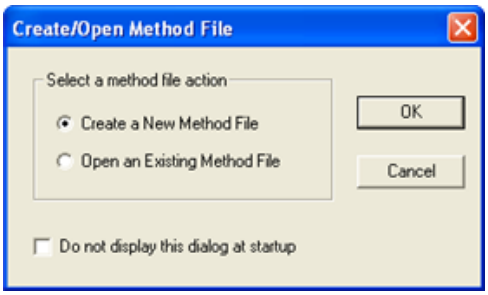
Calibration Block Report Format



Item	Description
Print Text Report Only/ Print Text and Curves	Selects whether the Workstation prints only a text report or prints the calibration curves when a Calibration Block Report is printed. Calibration Block Reports are printed when a Print Calib sample type is used in a SampleList or RecalcList (from System Control/Automation).
Show Outliers on Curve	If checked, prints the excluded points on the calibration curve.
Amount Units	Up to 10 characters Labels the amount units used in the calibration block report.

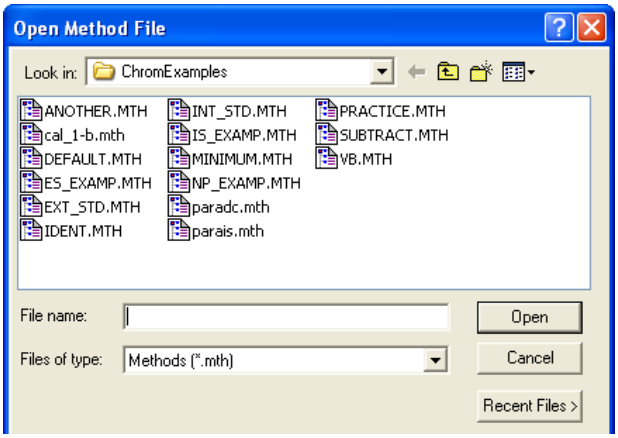
Method Builder Dialog Boxes

Create/Open Method File Dialog Box



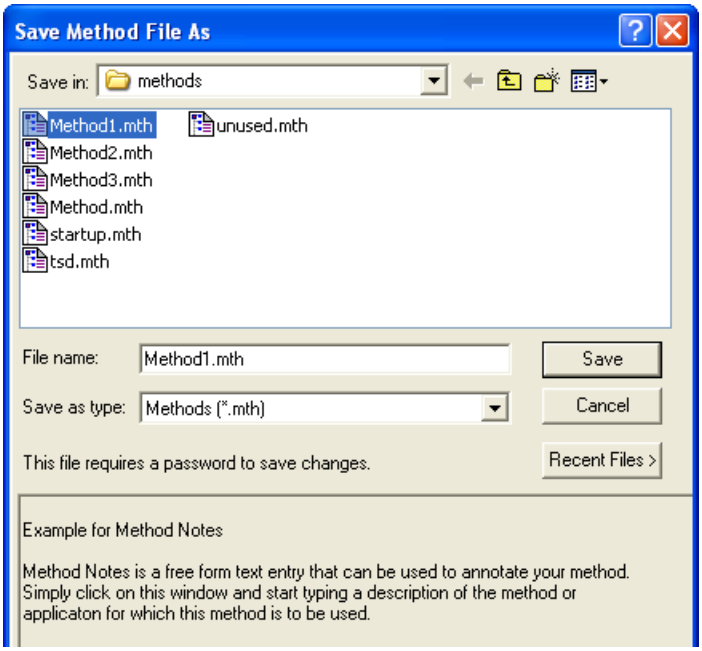
Item	Description
Select a method file action	If Create a New Method File is selected, then Method Builder is started to guide you through adding any hardware modules or post-run processing to a new Method file. If Open Existing Method File is selected, then the Open Method File dialog box is displayed for selecting the Method file to open.
Do not display this dialog at startup	When not checked, this dialog box is always displayed whenever the Method Builder application is started. When checked, this dialog box is not displayed. To redisplay the dialog box at startup, select Prompt for Action at Startup from the Method Builder File menu.
OK	Either starts Method Builder to configure a new method file or displays the Open Method File dialog box to select an existing Method file to open.
Cancel	Cancels the Method file action and closes the dialog box.

Open Method File Dialog Box



Item	Description
Look in	Lists the available folders and files. To see how the current folder fits in the hierarchy on your computer, click the down arrow. To see what's inside a folder, click it. The box below shows the folders and files in the selected location. You can also double-click a folder or file in that box to open it. To open the folder one level higher, click the “up arrow” button on the toolbar.
File list	Lists the folders and files in the selected location. To see what's inside a folder, double-click it. You can also use the Look In box to see the hierarchy of folders. To open the folder one level higher, click the “up arrow” button on the toolbar.
File name	Shows the currently selected file.
Files of type	Restricts the list of files to only those matching the selected type.
Recent Files	Click on this button to display a list of recently selected files. When you select a file from this list, it’s name is displayed in the File name box.
Notes	When checked, displays any notes and/or revision log associated with the currently selected file.
Open	Opens the selected file.
Cancel	Cancels file selection.

Save Method File As Dialog Box



Item	Description
Save in	Lists the available folders and files. To see how the current folder fits in the hierarchy on your computer, click the down arrow. To see what's inside a folder, click it. The box below shows the folders and files in the selected location. You can also double-click a folder or file in that box to open it. To open the folder one level higher, click the “up arrow” button on the toolbar.
File list	Lists the folders and files in the selected location. To see what's inside a folder, double-click it. You can also use the Save In box to see the hierarchy of folders. To open the folder one level higher, click the “up arrow” button on the toolbar.
File name	Shows the currently specified file.
Save as type	Specifies the type of file to save.
Recent Files	Click on this button to display a list of recently selected files. When you select a file from this list, it’s name is displayed in the File name box.
Notes	Displays any notes and/or revision log associated with the currently selected file.
Save	Saves the file with the specified name.
Cancel	Cancels file saving.

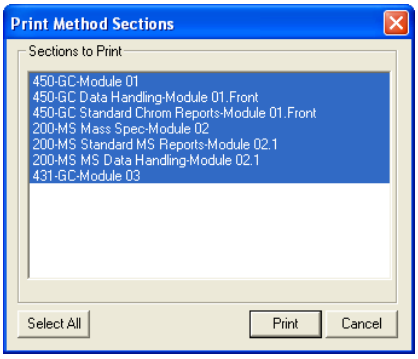
Add Password Dialog Box

Item	Description
Enter New Password	Enter password to be used in this box. Asterisks will appear as you type it.
Re-enter New Password	Enter password again. This password will be compared to the previously entered one to guard against typing errors.
OK	Applies the password to the Method and closes the dialog box.
Cancel	Closes the dialog box without applying the password to the Method.

Change Password Dialog Box

Item	Description
Enter Current Password	Enter the password currently used to protect the Method.
Enter New Password	Enter password to be used in this box. Asterisks will appear as you type it. If you leave this box blank, password protection will be removed from the Method.
Re-enter New Password	Enter password again. This password will be compared to the previously entered one to guard against typing errors.
OK	Applies the new password to the Method and closes the dialog box.
Cancel	Closes the dialog box without changing the password to the Method.

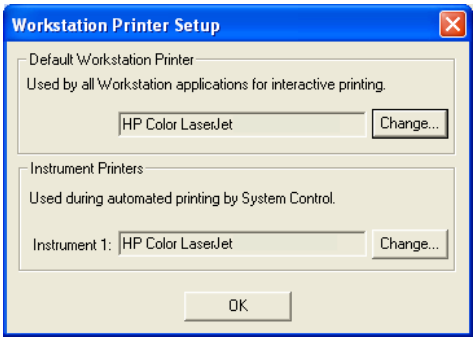
Print Method Sections Dialog Box



Item	Description
Sections to Print	Lists the sections of the Method. Selected sections will be printed. To print only certain Method sections, click on each section to print, then click on Print.
Select All	Selects all sections in the Method.
Print	Prints selected sections of the current Method and closes the dialog box.
Cancel	Closes the dialog box without out printing sections of the current Method.

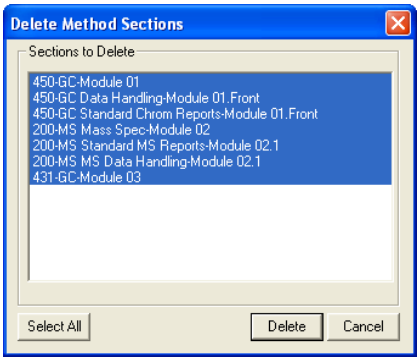
Star Printer Setup Dialog Box

This dialog box is used to specify the printers that will be used by Varian MS Workstation applications both interactively and during automation.



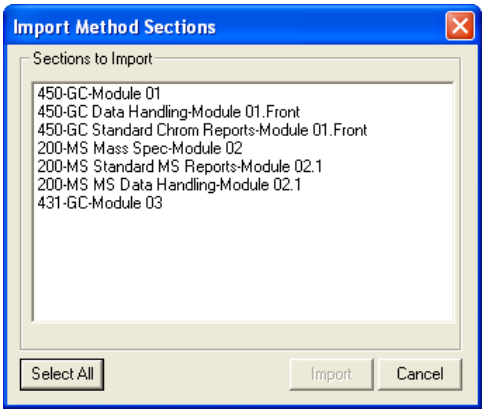
Item	Description
Default Star Printer	Displays the printer that is used when printing interactively from Varian MS Workstation applications. Click on the Change button to select a different printer.
Instrument Printers	Displays the printer that is used when printing under automation from System Control. A separate printer can be configured for each instrument (up to four). Click on the Change button to select a different printer for each instrument.

Delete Method Sections Dialog Box



Item	Description
Sections to Delete	Lists the sections of the Method. Selected sections will be deleted. To delete only certain Method sections, click on each section to delete, then click on Delete.
Select All	Selects all sections in the Method.
Delete	Deletes selected sections of the current Method and closes the dialog box.
Cancel	Closes the dialog box without out deleting sections of the current Method.

Import Method File Sections Dialog Box

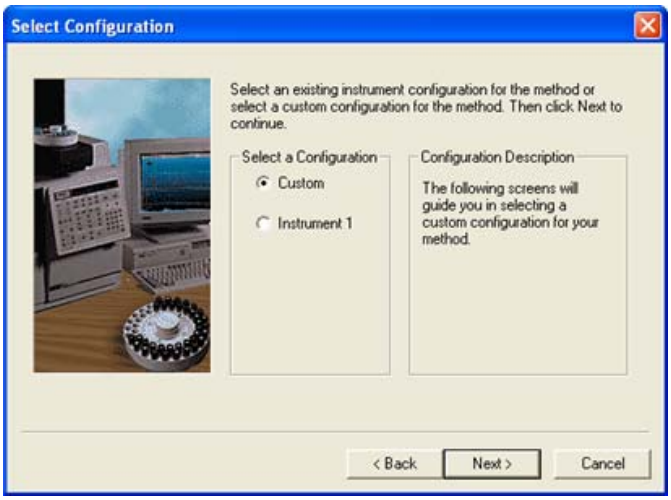


Item	Description
Sections to Import	Lists the sections of the Method. Selected sections will be imported. To import only certain Method sections, click on each section to import, then click on Import.
Select All	Selects all sections in the Method.
Import	Imports selected sections to the Method being edited and closes the dialog box.
Cancel	Closes the dialog box without out importing sections into the Method.

Method Builder Wizard

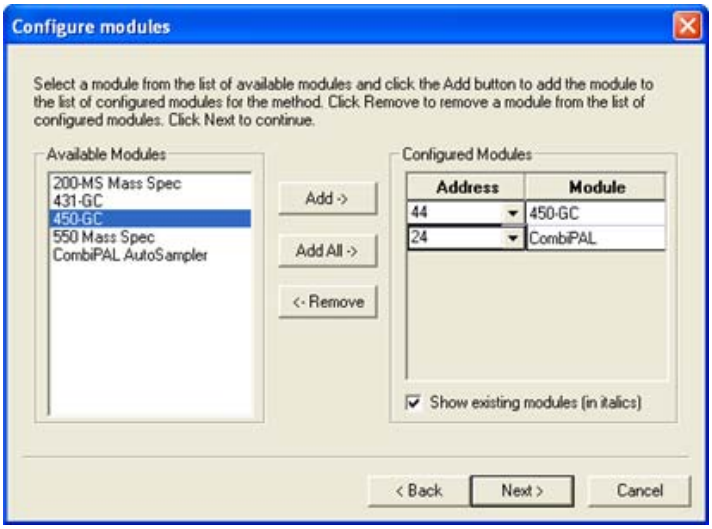
The Method Builder Wizard guides you through the process of creating a new Method or adding instrument control or post-run processing sections to an existing Method. You are prompted for information about the instrument on which you will be running the Method, the detectors whose data you wish to process, and the post-run applications that you wish to include in your Method. When finished, you can review the sections that are added to your Method before continuing.

Select Configuration



Item	Description
Select a Configuration	Select Custom in order to add any configuration of hardware modules to the Method file. Select the Instrument button in order to add only the hardware modules for that instrument configuration to the Method file. The Instrument configuration is the configuration of hardware modules and the associated Varian MS Workstation bus address defined by the user in the System Control application. The Instrument configuration is not available until the user has configured the hardware modules for the Instrument in System Control and has exited the Configuration screen of System Control or closed the System Control application.
Configuration Description	If you select the Instrument configuration, then a list of the hardware modules and the address of each module on the Varian MS Workstation bus is displayed for the selected Instrument.
Back	Displays the Introduction screen for the Star Assistant.
Next	Displays the next step of the Star Assistant.
Cancel	Closes the Star Assistant. Nothing is added to the Method file.

Configure Modules

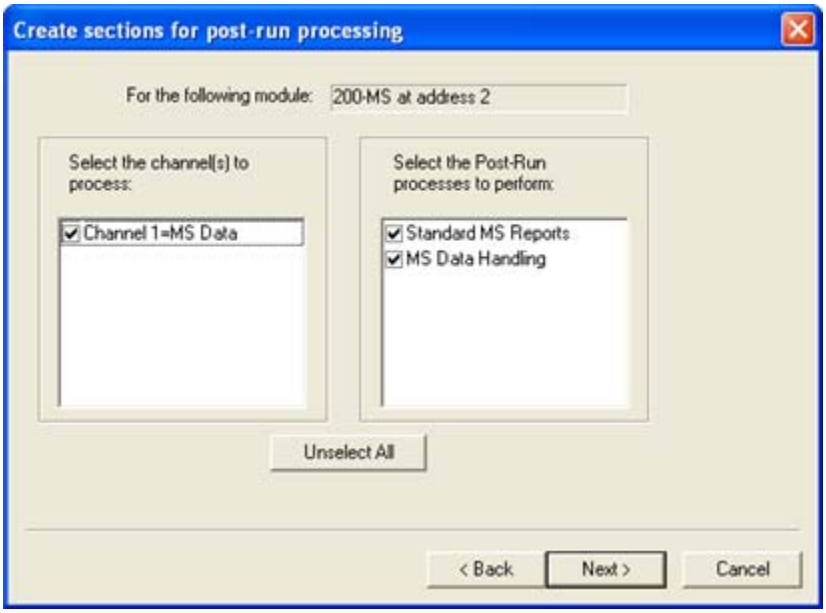


Item	Description
Available Modules	Lists the hardware modules that can be configured.
Configured Modules	Lists the hardware modules configured in the Method file. The modules are listed in the order they are added.
Add	Adds the selected hardware module from the Available Modules list to the Configured Modules list. The Varian MS Workstation bus address is automatically assigned. However, the address can be reassigned by selecting the drop-down arrow for the address in the Configured Modules list.
Add All	Adds one of each hardware module in the Available Modules list to the Configured Modules list. The Varian MS Workstation bus address is automatically assigned. However, the address can be reassigned by selecting the drop-down arrow for the address in the Configured Modules list.
Remove	Removes one or more selected hardware modules from the Configured Modules list. Selecting the header for either the Address or Module column removes all of the added hardware modules from the Configured Modules list.
Show existing modules	If checked, any existing hardware modules in the Method file are listed in italics in the Configured Modules list. If not checked, any existing hardware modules are not listed in the Configured Modules list. The addresses of existing hardware modules cannot be changed in the Configured Modules list. The addresses can only be changed from the Method Parameters window for that hardware module.
Back	Displays the Select Configuration screen for the Star Assistant.
Next	Displays the next step of the Star Assistant.
Cancel	Closes the Star Assistant. Nothing is added to the Method file.

Select Detectors for Post-Run Processing

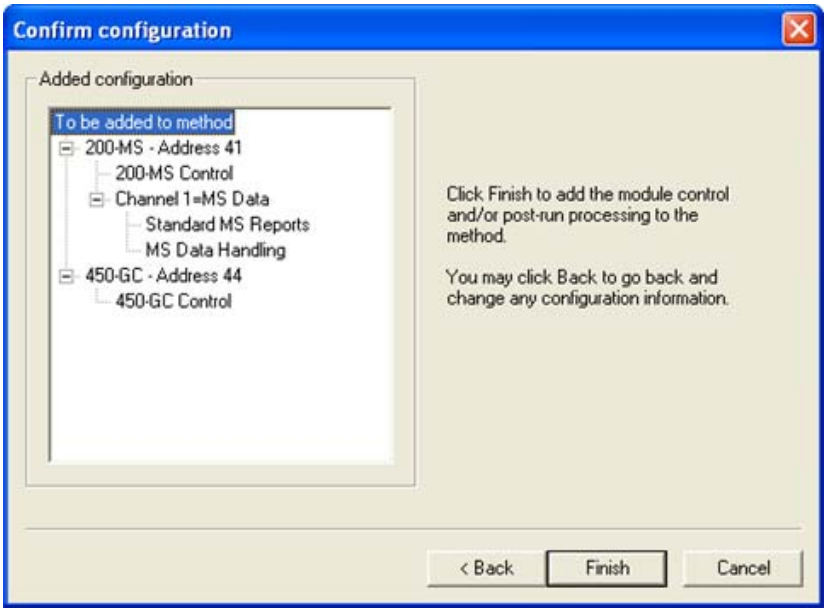
Item	Description
Detector Modules	Specifies the detectors for which you want to add post-run processing to the Method file. If the detector is checked, subsequent steps allow you to configure the post-run processing for the detector.
Select All	When clicked, all of the listed Detector Modules are checked and configured for post-run processing. If all of the Detector Modules are checked, then the button text is changed to Unselect All.
Back	Displays the previous screen for the Star Assistant.
Next	Displays the next step of the Star Assistant.
Cancel	Closes the Star Assistant. Nothing is added to the Method file.

Create Sections for Post-Run Processing



Item	Description
For the following module	Specifies the detector module and address for which post-run processing is added. This Star Assistant screen is repeated for each detector modules selected in the previous Select Detectors for Post-Run Processing screen.
Select the channel(s) to process	If checked, the selected channel is configured for post-run processing. When this Star Assistant screen is first displayed, the default channel for the detector module is selected. The selected (or checked) channels apply to all of the selected post-run processing.
Select the Post-Run processes to perform	If checked, the selected post-run processing is added to the Method file for all of the checked channels. Any existing post-run processing in the Method file is not overwritten so you may safely select any combination of channel and post-run processing for the detector module.
Select All	When clicked, all of the listed detector channels are checked and all of the listed post-run processing are checked. If all of the detector channels and post-run processing are checked, then the button text is changed to Unselect All.
Back	Displays the previous screen for the Star Assistant.
Next	Displays the next step of the Star Assistant.
Cancel	Closes the Star Assistant. Nothing is added to the Method file.

Confirm Configuration



Item	Description
Added Configuration	Displays the hardware modules, hardware control methods, and any post-run processing for detector modules that are to be added to the Method file. Any existing hardware control methods and post-run processing are not overwritten and are not listed in the configuration to be added.
Back	Displays the previous screen for the Star Assistant.
Finish	After you have confirmed the configuration to be added to the Method file, clicking Finish will add the configuration to the Method file. The Method Directory pane for the Method will be updated to reflect the added configuration.
Cancel	Closes the Star Assistant. Nothing is added to the Method file.

Standard GC Reports Command Reference

File Menu

Menu Item	Description
Open	Displays the Open Data File dialog box.
Print	Displays the Print dialog box.
Convert (ASCII)	Converts the text results report into an ASCII file. The name of the ASCII file is based on the data file name, with the channel number appended to it. The ASCII file ends with a ".txt" extension.
Printer Setup	Displays the Printer Setup dialog box.
Exit	Quits the Standard Report application.

Search Menu

Displayed when the results window is active.

Menu Item	Description
Find	Displays the Find dialog box.
Find next	Repeats the search last performed with the Find dialog box.

Font Menu

Displayed when the results window is active.

Menu Item	Description
Small	Uses a small font to display the results report. For display only.
Medium	Uses a medium font to display the results report. For display only.
Large	Uses a large font to display the results report. For display only.

View Menu

Displayed when the chromatogram window is active.

Menu Item	Description
Change Plot Color	Displays a dialog box allowing you to select a color for the chromatogram plot. This plot color is used in the display only.

Options Menu

Menu Item	Description
Report Title	Displays the Report Title dialog box.
Chromatogram	Displays the Chromatogram Options dialog box.
Results	Displays the Results Options dialog box.
Save Changes to Data File	Saves any changes made to the report title, chromatogram options or results options to the currently open data file. The next time you display the data file in the standard report application, these new settings will be used.

Windows Menu

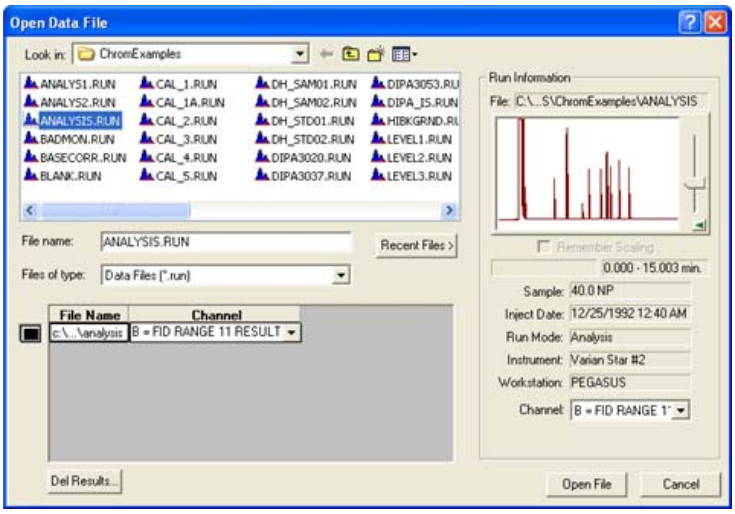
Menu Item	Description
Tile	Arranges the chromatogram and results windows in a tiled fashion.
Cascade	Arranges the chromatogram and results windows in an overlapped fashion.
Arrange Icons	If either the chromatogram window or results window (or both windows) are iconized, the icons are arranged in the report window.
Chromatogram Window	Activates the chromatogram window.
Results Window	Activates the results window.

Help Menu

Menu Item	Description
Help Topics	Displays the help.
Product Support Web Site	If you have Internet access and a web browser installed on your computer, this option will automatically open the varian, inc. Web Site. Here you will find the latest software and documentation updates for the Varian, Inc. suite of products, along with additional notes, tips, and answers to frequently asked questions.
About Report	Displays the About Box for the Standard Report application. The About Box contains information about the software version, installation information, and a list of the instrument control modules that you have installed.

Standard GC Reports Dialog Boxes

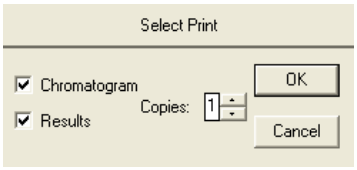
Open Data File Dialog Box



Item	Description
Look in	Lists the available folders and files. To see how the current folder fits in the hierarchy on your computer, click the down arrow. To see what's inside a folder, click it. The box below shows the folders and files in the selected location. You can also double-click a folder or file in that box to open it. To open the folder one level higher, click the “up arrow” button on the toolbar.
File list	Lists the folders and files in the selected location. To see what's inside a folder, double-click it. You can also use the Look In box to see the hierarchy of folders. To open the folder one level higher, click the “up arrow” button on the toolbar.
File name	Shows the currently selected file.
Files of type	Restricts the list of files to only those matching the selected type.
Recent Files	Click on this button to display a list of recently selected files. When you select a file from this list, it’s name is displayed in the File name box.
Run Information	Shows information about the currently selected file, including a thumbnail view of the chromatogram. If you are looking at several files and you wish to use a fixed attenuation in the thumbnail display, check the Remember Scaling box. Select the channel you wish to open in the Channel selection box. When you do, the chromatogram thumbnail and Run Information is updated.

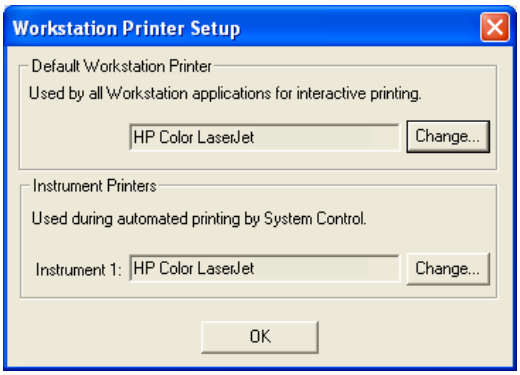
Item	Description
Del Results	Allows you to delete results from the currently select channel of the currently selected data file. This button does not appear if it has been disabled from the Varian MS Workstation Security Administration application.
Open File	Opens the selected data file using the selected channel.
Cancel	Cancels file selection.

Print Dialog Box



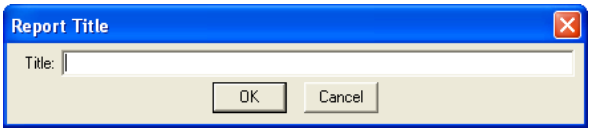
Item	Description
Chromatogram	When checked, prints the chromatogram as part of the report.
Results	When checked, prints the results as part of the report.
Copies	Sets the number of copies of the report to be printed.

Printer Setup Dialog Box



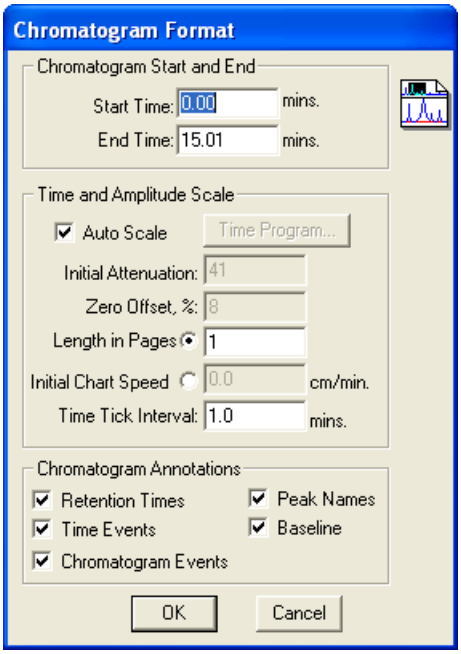
Item	Description
Default MS Workstation Printer	Displays the printer that is used when printing interactively from Varian MS Workstation applications. Click on the Change button to select a different printer.
Instrument Printers	Displays the printer that is used when printing under automation from System Control. A separate printer can be configured for each instrument (up to four). Click on the Change button to select a different printer for each instrument.

Title Dialog Box



Item	Description
Title	Assigns a title to the report. The title appears in both the chromatogram and results portion of the printed report.

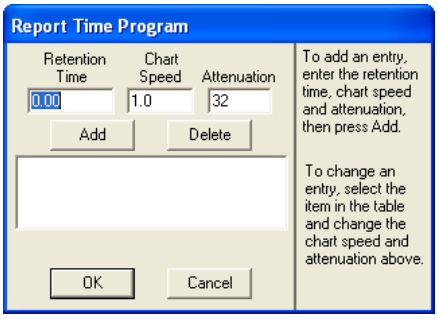
Chromatogram Options Dialog Box



Item	Description
Start Retention Time, mins	0.00 to 1440.00 Specifies a start time after injection for the chromatogram display and printout.
End Retention Time, mins	0.01 to 1440.00 Specifies an end time for the chromatogram display and printout. If the End Retention Time is greater than the actual end time in the data file, the actual end time is used.

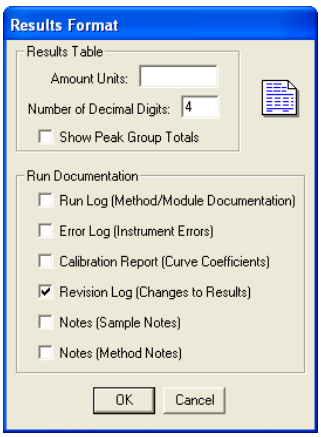
Item	Description
Initial Attenuation	1 to 4096 Sets the initial scaling of the display or printout. Attenuation is relative to the maximum full scale value of the detector. An attenuation of 1 scales the chromatogram so that a signal 1/4096th of the detector's full scale is the largest signal that will be printed. The attenuation can be changed to other values at various times by time programming. The initial attenuation value is ignored if you select Auto Scale.
Zero Offset, %	-100 to 100 Sets the zero point of the displayed or printed chromatogram as a percentage of the full page. Larger values let you record negatively drifting baselines or negative chromatographic peaks. The zero offset value is ignored if you use Auto Scale.
Length in Pages	0 to 9 Sets the number of pages used to print a chromatogram. This option takes precedence over the chart speed value. The chart speed is calculated by dividing the total length in pages by the run time.
Initial Chart Speed, cm/min	0.0 to 30.0 Sets the initial chart speed for the printout. This speed does not change unless you time program the chart speed. Set the Length in Pages to 0 to use this option.
Minutes per Tick	0.0 to 10.0 Sets the interval between time tick marks on the printout.
Auto Scale	If checked, adjusts the attenuation and zero offset so that the chromatogram fills the screen or page.
Time Events	If checked, annotates the right margin of the chromatogram to show when time events occurred. Shows when peak width (WI), inhibit integrate (II), solvent reject (SR), group (GR), valley baseline (VB), chart speed (CS), and attenuation (ATT) changes occurred.
Chromatogram Events	If checked, annotates the chromatogram with tick marks that denote peak event for peak starts, peak ends, apices, and valley points.
Retention Times	If checked, annotates the chromatogram with the retention times for all detected peaks.
Peak Names	If checked, displays peak names for identified peaks.
Baseline	Draws baseline segment lines under the peaks.
Edit Time Program...	Opens the Report Time Program dialog box to edit a report time program.

Report Time Program Dialog Box



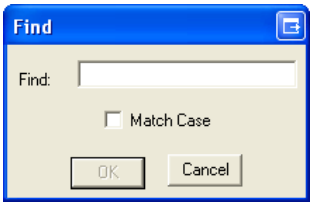
Item	Description
Retention Time	0.00 to 1440.0 Sets the start time for the selected event.
Chart Speed	0 .1 to 30.0 Sets the program chart speed.
Attenuation	1 to 4096 Sets the program attenuation.. Attenuation is relative to the maximum full scale value of the detector. An attenuation of 1 scales the chromatogram so that a signal 1/4096th of the detector's full scale is the largest signal that will be printed.
Add	Adds the active parameters to the program list. To add a change in chart speed or attenuation to the report time program.
Delete	Deletes the highlighted line in the program. To delete a line in the report time program, canceling that change in chart speed or attenuation.

Results Options Dialog Box



Item	Description
Units	Any units, up to 10 characters Assigns a name for the units used in the results report.
Number of Decimal Digits	0 to 6 Sets the number of digits in which results are to be expressed.
Run Log	If checked, includes the method and the Time Events Log at the end of the report. Entries in the Time Events Log correspond to the actual times when the events occurred.
Error Log	Includes error messages that occurred during the run at the end of the report. Error messages generated by post-run Data Handling are always printed whether the error log option is active or not.
Calibration Report	Includes the text of the calibration block report as part of the results report.
Notes	Includes the notes you entered when you made the injection (original notes) and when you recalculated (appended notes) as part of the report.

Find Dialog Box



Item	Description
Find	Sets which string of characters the Workstation will find
Match Case	If checked, tells Report to find only character strings with the same use of upper and lower case

Standard GC Reports Format Descriptions

Results Report

The following is an example of a results report generated from an analysis run. The exact format of your results reports may vary depending on the following parameters:

- Options set in the Results Format portion of the Method
- The type of run being performed (blank baseline, calibration, analysis, or verification)
- The peak measurement type (area, height or square root of height)
- The calculation type (percent, normalized percent, internal standard or external standard)
- The presence of an RRT peak, designated in the peak table (which determines whether relative retention time is displayed)

The format of the ASCII text file generated when ASCII file conversion is performed is identical to the format in the printed report.

Following this example is a legend of the fields that appear in the report.

Title   : Title

Run File   : Data File name

Method File : Method File name

Sample ID   : Sample name

Injection Date: Date/Time   Calculation Date: Date/Time

Operator   : Operator Name   Detector Type: Detector Type/Range

Workstation: Volume Label   Bus Address : module bus address

Instrument : Instrument Name   Sample Rate : Sample Rate (Hz)

Channel   : Channel ID/Name   Run Time   : Run Time (min)

********** Star Chromatography Software
****

Run Mode   : Run Mode

Peak Measurement: Measurement Type

Calculation Type: Calculation Type

Peak No.	Peak Name	Result (units)	Standard Peak Name	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel. Ret. Time	Width Sep. Code	1/2 (sec)	Group	Status Codes
1	2-Octanone	INT STD	2-Octanone	5.677	0.004	4270	1.000	BB	1.5	1	SR
2	1-Octanol	7.5438	2-Octanone	6.996	0.022	749	1.232	BB	3.3	1	
3	n-Decane	30.1366	2-Octanone	7.514	0.002	1511	1.324	BB	1.6	1	C
4	2,6-dimetphe	INT STD	2,6-dimetphe	8.479	0.001	2414	1.494	BB	1.7	2	S
5	n-Dodecane	16.8705	2,6-dimetphe	8.998	-0.005	4608	1.585	BB	1.8	2	C
6	2,4-dimetani	16.8549	2,6-dimetphe	9.325	-0.004	3545	1.643	BB	1.8	2	C
7	n-Tridecane	16.8653	2,6-dimetphe	10.856	-0.006	3569	1.912	BB	1.9	2	C
	Group 1	37.6804			0.028	6530					
	Group 2	50.5907			-0.014	14136					
	Totals:	88.2711			0.014	20666					

Status Codes:

R - Reference peak

* - No result could be calculated; check calibration curve

M - Missing peak

C - Out of calibration range

S - Internal Standard peak

U - User-defined peak endpoint(s)

Total Unidentified Counts :   0 counts

Detected Peaks: 7   Rejected Peaks: 0   Identified Peaks: 9

Standard Peak Amounts:

2-Octanone   Amount = 12

2,6-dimetphe   Amount = 12

Multiplier: 1   Divisor: 1

Baseline Offset: -20 microVolts

Noise (used): 1 microVolts - monitored before this run

Manual injection

Run Log:

```
[Module Run Logs]
Time Events:
[Data Handling Time Events]
Error Log:
[Module Error Logs]
Calibration Report:
[Calibration Report Text]
Revision Log:
[Revision Log]
Original Notes:
[Original Note Text]
Appended Notes:
[Recalc Note Text]
********************************************************************************
```

Item	Description
Title	Set in the Print Options portion of the Report section of the Method.
Run File	The file name of the Data File containing the results.
Method File	The file name of the Method used to generate the current results. This may differ from the Method used when the data was first generated.
Sample ID	Set in the SampleList when the injection was performed.
Injection Date	The date and time of the injection.
Calculation Date	The data and time of the most recent calculation.
Operator	Set in the System Control Instrument Parameters dialog box. This is the name of the operator at the time of the injection.
Detector Type	The type of the detector used to collect the data (for example, 9050, 9065, or ADC Board).
Workstation	The name of the Workstation on which the data was collected. The Workstation name is the volume label of the hard disk on which System Control is running at the time of the injection.
Bus Address	The bus address of the detector used to collect the data.
Instrument	Set in the System Control Instrument Parameters dialog box. This is the name of the instrument at the time of the injection.
Sample Rate	The rate (frequency) of the data stored in the Data File.
Channel	The channel ID corresponding to the data for which results are displayed.
Run Time	The length of the run in minutes. Set in the instrument control Method section corresponding to the detector that collected the data.
Run Mode	Set in the SampleList or SampleLog (in System Control) or Reintegration List (in Interactive Graphics). Either Blank Baseline, Analysis, Calibration or Verification. If blank baseline subtraction has occurred (set in the Integration Parameters window in the Data Handling Method section), it is indicated on this line.
Peak	Set in the Integration Parameters window in the Data Handling

Item	Description
Measurement	Method section. Either Area, Height or Square Root of Height.
Calculation Type	Set in the Integration Parameters window in the Data Handling Method section. Either Percent, Normalized Percent, Internal Standard or External Standard. If results have been normalized (set in the Integration Parameters window in the Data Handling Method section), it is indicated on this line.
Peak No.	The number of the peak in the results table.
Peak Name	Set in the Peak Table Window in the Data Handling Method section. Peak names are displayed for peaks that have been identified as being in the peak table.
Result (units)	The calculated results. The units (set in the Results Format portion of the Data Handling Method section) are displayed in the results column header.
Standard Peak Name	This column is displayed when internal standard calibration is used and there exists more than one standard peak. This refers to the name of the standard peak used for the given non-standard peak.
Ret. Time	The actual retention time of the peak, in minutes.
Time Offset (min)	The amount of time, in minutes that the actual retention time differs from the retention time for the peak in the peak table. The retention time in the peak table is automatically updated with the actual retention time to account for peak drift.
Area (counts)	The measured peak size. This will either be the area, height or square root of height, depending upon the peak measurement type (set in the Integration Parameters window in the Data Handling Method section). The column header will reflect the appropriate measurement type.
Rel. Ret. Time	Reported when an RRT peak has been designated in the peak table (in the Data Handling Method section). The Workstation calculates relative retention times from the retention time of the RRT peak and the unretained peak time (set in the Define Peak Windows dialog box accessed from the peak table).
Sep. Code	A two letter code indicating the relationship of the peak start and end to the baseline. Possible separation codes are BV: Baseline to valley BB: Baseline to baseline VB: Valley to baseline VV: Valley to valley TS: Separated Tangent Peaks TF: Fused tangent peaks GR: Group Peak BM: Baseline to mended end MB: Mended end to baseline MM: Mended end to mended end MV: Mended end to valley VM: Valley to mended end
Width 1/2 (sec)	The width of the peak at half its height.

Item	Description
Group	This column is displayed when the Show Peak Group Totals checkbox is checked in the Results Format portion of the Report Method section. The group number for each peak is set in the peak table in the Data Handling Method section.
Status Codes	A code or codes specific to a peak in the results table. Possible status codes are R: Reference Peak (designated in the peak table) *: No result can be calculated, check the calibration curve. +: More than one result can be calculated, the first solution is displayed in the results field. Check your calibration curve or use a lower order curve fit (specified in the peak table). V: Peak fails verification (verification runs only) M: Missing peak (if Report Missing Peaks is set in the Integration Parameters Window in the Data Handling section of the Method) C: Result out of calibration range, check the calibration curve and the range tolerance setting in the Method. S: Internal Standard Peak (designated in the peak table for internal standard and normalized percent calculations only) U: User-defined peak endpoint (the peak size is affected by an endpoint that was manually placed in Interactive Graphics).
Total Unidentified Counts	The total number of counts accounted for by peaks not identified in the peak table.
Detected Peaks	The total number of peaks detected during integration. Peak detection is affected by parameters set in the Integration Parameters Window in the Data Handling Section of the Method.
Rejected Peaks	The total number of detected peaks that were rejected based on values set in the Integration Parameters Window in the Data Handling Section of the Method.
Identified Peaks	The total number of detected peaks that were identified in the peak table.
Standard Peak Amounts	Set in the SampleList or SampleLog (in System Control) or the Reintegration List (in Interactive Graphics). This is used with Normalized Percent and Internal Standard calculations and identifies the amount of the Standard Peak(s) (designated in the Peak Table Window in the Data Handling Section of the Method).
Multiplier	Set in the SampleList or SampleLog (in System Control) or the Reintegration List (in Interactive Graphics). The result for each peak is multiplied by this value.
Divisor	Set in the SampleList or SampleLog (in System Control) or the Reintegration List (in Interactive Graphics). The result for each peak is divided by this value.
Baseline Offset	The distance the chromatographic signal is above or below zero at the start of the run. Baseline offset is measured in microunits (units are volts or absorption units, depending upon the detector). The baseline offset is equivalent to the amplitude of the first data point in the Data File.
Noise	Noise is the peak-to-peak noise measured in microunits (units are volts or absorption units, depending upon the detector).

Item	Description
	The noise used by Data Handling depends upon the noise options set in the Integration Parameters Window in the Data Handling section of the Method. The report includes the noise value for this run, and the noise value actually used, if it is different.
Manual injection (injection information)	Indicates the type of injection device used (for example, manual injection, 8200 AutoSampler, or AI-200 AutoSampler), and the rack, vial and injection volume, if appropriate.
Run Log	The Run Log is included in the report if the Run Log checkbox is checked in the Results Format portion of the Report section of the Method. The Run Log is the instrument control Method that was used in the run that generated the Data File. For 3400 and 3600 GCs, it is the Method as it was downloaded before the run began. The 3400 or 3600 Event Log (included in the Run Log) will describe any changes that occurred after run start. For all LC modules, the Run Log is the Method that was actually executed on the LC module itself. Any changes that occurred during the execution of the Method will be incorporated into the Run Log. Also included with the Run Log is information from the Module Information Log, which can be edited in System Control on a per-module basis.
Time Events	Data Handling timed events (programmed in the Time Events Window in the Data Handling Section of the Method) are listed with the times that they actually occurred.
Error Log	The Error Log is included in the report if the Error Log checkbox is checked in the Results Format portion of the Report section of the Method. The Error Log is a list of errors that occurred during the run that generated the Data File.
Calibration Report	The Calibration Report is included in the report if the Calibration Report checkbox is checked in the Results Format portion of the Report section of the Method. The Calibration Report is the text portion of the Calibration Block Report for the Method used to calculate results. It includes the calibration responses and curve coefficients for each peak.
Revision Log	The Revision Log is included in the report if the Revision Log checkbox is checked in the Results Format portion of the Report section in the Method. The Revision Log contains the date/time and Method name used every time a recalculation is performed on the Data File. Results deletion is also documented in the Revision Log. Documentation of recalculations can be disabled from the Security Administration application.
Original Notes	The Original Notes are included in the report if the Notes checkbox is checked in the Results Format portion of the Report section of the Method. The Original Notes are the notes set in the SampleList in System Control when the injection was performed that generated the Data File.
Appended Notes	The Appended Notes are included in the report if the Notes checkbox is checked in the Results Format portion of the Report section of the Method. The Appended Notes are the notes set in the SampleLog (in System Control) or in the Reintegration List (in Interactive Graphics) during the most recent recalculation performed on the Data File.

Verification Report

Below is an example of a results report generated from a verification run. The exact format of your verification reports may vary depending on the following parameters:

Options set in the Results Format portion of the Method

- The type of run being performed (blank baseline, calibration, analysis, or verification)
- The peak measurement type (area, height or square root of height)
- The calculation type (percent, normalized percent, internal standard or external standard)
- The presence of an RRT peak, designated in the peak table (which determines whether relative retention time is displayed)

The format of the ASCII text file generated when ASCII file conversion is performed is identical to the format in the printed report.

Following this example is a legend of the fields that appear in the report. Only those fields that differ from the Analysis Report are listed. See the Results Report Format Description for a listing of the additional fields.

```
                              Verification Report

Title       : Title
Run File    : Data File name
Method File : Method File name
Sample ID   : Sample name
Injection Date:  Date/Time            Calculation Date: Date/Time
Operator   : Operator Name          Detector Type: Detector Type/Range
Workstation: Volume Label           Bus Address  : module bus address
Instrument : Instrument Name        Sample Rate  : Sample Rate (Hz)
Channel    : Channel ID/Name        Run Time     : Run Time (min)
********** Star Chromatography Software
************************************

Run Mode        : Verification
Peak Measurement: Measurement Type
Calculation Type: Calculation Type
Level           : Verification Level
Tolerance       : 100.0%
                   Expected  Calculated        Ret.   Time
Peak     Peak       Result     Result   Dev.  Time   Offset    Area   Status
 No.     Name         ()         ()       %    (min)   (min)  (counts) Codes
 --- ------------ ---------- ---------- ----- ------- ------- -------- ------
   1 Peak 1.841          N/A    INT STD   0.0   1.841  -0.000   220494 S
   2 Peak 2.004       1.0000                    2.004                  VM
   3 Peak 2.205       1.0000                    2.205                  VM
   4 Peak 2.756       1.0000     2.4122 141.2   2.754   0.000   102519 CV
   5 Peak 3.297       1.0000     2.0112 101.1   3.298   0.001  1212397 RV
   6 Peak 3.798       1.0000     2.0191 101.9   3.799  -0.000   493782 V
   7 Peak 4.791       1.0000     1.9279  92.8   4.789  -0.001   700782
   8 Peak 5.125       1.0000     4.7624 376.2   5.104  -0.000   328998 CV
   9 Peak 5.580       1.0000     1.4435  44.3   5.586  -0.001   297265
```

```
 --- ------------ ---------- ========== ----- ------- ======= ======== ------
     Totals:                   14.5762               -0.002  3356238
Status Codes:
R - Reference peak
V - Out of verification tolerance
M - Missing peak
C - Out of calibration range
S - Internal Standard peak
Total Unidentified Counts :          0 counts
Detected Peaks: 7           Rejected Peaks: 0      Identified Peaks: 9
Standard Peak Amount:
2-Octanone       Amount = 12
Multiplier: 1          Divisor: 1
Baseline Offset: -20 microVolts
Noise (used): 1 microVolts - monitored before this run
Manual injection
********************************************************************************
*
```

Item	Description
Level	Set in the SampleList or RecalcList (in System Control) or in the Reintegration List (in Interactive Graphics). This corresponds to the concentration level used in the verification sample, which can be the same as one of the calibration levels, or can be between levels used in calibration. The value in the peak table at this level is assumed to be the amount of the compound used in the verification sample.
Tolerance	Set in the Verification dialog box accessed from the Peak Table Window in the Data Handling section of the Method. This is the maximum acceptable deviation percentage allowed before considering a peak to be out of tolerance.
Expected Result	This is the amount obtained from the peak table corresponding to the designated verification level.
Calculated Result	This is the result calculated from the calibration curve using the detector response from the verification run. If no drift has occurred in the system, and the amount of the compound in the verification sample is identical to the amount of the same compound in the calibration sample at the same level, then this value will be the same as the expected result.
Dev. %	The percentage that the calculated result deviates from the expected result. If this value is larger than the tolerance, then a verification failure occurs.

Standard GC Reports Toolbar

Main Toolbar

	Displays the Open Data File dialog box.
	Displays the Print dialog box.
	Converts the text results report into an ASCII file. The name of the ASCII file is based on the data file name, with the channel number appended to it. The ASCII file ends with a ".txt" extension..
	Displays the Find dialog box.
	Displays the Title dialog box.
	Displays the Chromatogram Options dialog box.
	Displays the Results Options dialog box.
	The Data File Quick Link button shows the current Data File. Use this Quick Link button to perform additional operations on the Data File.
	The Method Quick Link button shows the Method used for the most recent recalculation of the selected channel for the data file. Use this Quick Link button to view, edit or print this Method.
	This selection box contains all channels for the selected data file and allows you to switch between them without re-opening the file.