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Agilent Technologies

Varian, Inc. 2700 Mitchell Drive Walnut Creek, CA 94598-1675/USA

300 Series GC/MS and LC/MS Quadrupole Mass Spectrometer MS Workstation Version 6

Software Operation Manual



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Introduction

Overview

The Varian MS Workstation Version 6 software controls the 300 Series Quadrupole instruments, associated Varian chromatography modules and several modules from other vendors. Use this manual to maximize your application of the features.

Additional Manuals

300 Series Hardware Operation Manual

This manual, part number 3954912500, provides the necessary information for using, maintaining, and repairing your 300 Series System. This information is also available in Online Help.

MS Workstation Software Reference Manual

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

Data Acquisition with 3800 GC Control

This manual, part number 391473100, explains how to build methods, acquire data, and operate the 3800 GC with your Varian MS Workstation. This manual also describes the configuration of the 3800 GC for standard Ethernet communication with the System Control application.

Data Acquisition with LC Control

This manual, part number 391473200, describes the operation of the MS Workstation with Varian HPLC modules. It covers configuring an instrument for data acquisition, building a method, and running samples.

DIP/DEP Solids Probe Manual

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

Chromatography Hardware Manuals

Refer to the manuals of your chromatography modules.

MS Workstation Applications

Overview

The applications of the Varian MS Workstation Toolbar are: Methods, Data Files, SampleLists, RecalcLists, SequenceLists, and Reports. They are on the Varian MS Workstation Toolbar and in the Varian MS Directory. When you install other MS Workstation options, such as Star Finder and Star Custom Report Writer you can add those application buttons. The followingtgr4 is a brief introduction to the applications. Each is explained in detail in later sections.





System Control - Control Varian instruments including the 300 Series MS, HPLC, and GC modules. There are two main windows, the Configuration window, and the Data Acquisition and Control window.



Method Builder - Edit or create methods for the 300 Series MS, Varian HPLC, and GC chromatography modules.



Automation File Editor - Build SampleLists, RecalcLists, and SequenceLists for System Control automation. You may also build these Automation Files directly in System Control.



MS Data Review - Review chromatograms and spectra, do library searches, and review and process quantitation results.



Standard MS Report - Edit the standard MS report template.



Custom MS Report - Create custom report templates.



Security Administration - Select MS Workstation security options and passwords.



Data File Conversion - Convert older data files collected with Varian Ion Trap Mass Spectrometers to the current data file formats. Keep an archive of existing data with current data files for quick and easy reference.



DAT to MS Conversion - Convert Kodiak DAT files to MS Workstation XMS format.



Batch Reporting - Automatically print one or many reports by dragging data file names from the Explorer or My Computer window and dropping them onto the Batch Reports window. The reports are printed with the method last used to process the data files.



View/Edit Chromatograms - View and edit chromatographic data gathered by conventional HPLC and GC detectors. You may load up to 7 chromatograms, manually or automatically assign or re-assign chromatogram events, and generate new results.



Standard Chrom Reports - Display and edit the preferences for reports generated from traditional chromatography detectors such as UV/Vis or FID detectors. These reports may be viewed one-at-a-time.



Compound Set Editor - Create and edit sets of compounds in the MS Data Handling Method allowing activation or deactivation under automation.



Quick Start - Make a single LC/MS or GC/MS injection quickly. Do not use this for multiple injections. Refer to the Injecting Samples and Automation section for more information.



PolyView™ 2000 - View and process PDA data from your Varian HPLC Photo Diode Array detector.



Aurora PDA - View HPLC Photo Diode Array data in a 3D presentation.

MS Workstation Toolbar Options

Moving the Workstation Toolbar

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

The Workstation Toolbar Options Menu

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

	Move to Windows Task Bar	
	Show/Hide Applications on Toolbar	
	Enable/Disable Instrument Modules	
~	Application Descriptions	
-	Small Buttons on Toolbar	
	Run Application	
	Help on	
	Pick Data File for Quick Link Button	
	Pick Method for Quick Link Button	
	Help on Workstation Toolbar	
	Product Support Web Site	
	About Workstation Toolbar	
	Quit	

Move to Windows Taskbar

Display the Workstation Toolbar as a Windows Taskbar icon.

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

Show/Hide Applications on Toolbar

Select which MS Workstation applications to represent with icons on the Workstation Toolbar. The top list box shows applications displayed in the toolbar. The bottom list shows all installed applications not displayed. To remove an icon from the toolbar, select it from the top list and click Remove. To add an icon to the toolbar, select it from the bottom list and click Add.

Enable/Disable Instrument Modules

Select which MS Workstation instrument modules are available. Available instrument modules are in System Control, if they are connected and turned on.

elect instrument modules you wish to disable.		Select instrument modules you wish to enable.
2000 Mass Spec 212-LC Solvent Delivery System	<u>^</u>	2002 Micro-GC 2003 Micro-GC
3800 GC 3900 GC	>>Disable>>	3400 GC 3600 GC
800 Interface Box		39XL GC
8200 AutoSampler ADC Board		4900 Micro GC 9001 Solvent Delivery System
CombiPAL AutoSampler		9002 Solvent Delivery System
Mistral Column Oven ProStar 220 SDM		9010 Solvent Delivery System 9012 Solvent Delivery System
ProStar 230 Inert SDM		9050 UV-Vis Detector
ProStar 230 SDM		9100 AutoSampler
ProStar 240 Inert SDM ProStar 240 SDM		9200 Prospekt 9300 AutoSampler
ProStar 310 UV-Vis Detector		AI-200 AutoSampler
ProStar 325 UV-Vis Detector ProStar 330 PDA Detector	< <enable<<< td=""><td>ProStar 520 Column Oven</td></enable<<<>	ProStar 520 Column Oven
ProStar 335 PDA Detector		
ProStar 363 Fluorescence Detector		
ProStar 400 AutoSampler ProStar 410 AutoSampler		
ProStar 420 AutoSampler	×	

The list on the left has all the instrument modules currently installed and enabled in the MS Workstation. The list on the right shows all instrument modules that are installed but not enabled. To disable an instrument module, select it from the list on the left and click **Disable**. To enable an instrument module, select it from the list on the right and click **Enable**.

Small Toolbar Buttons



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

Application Descriptions

Pause the cursor over an icon or a button to display a description.

Run Application

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

Pick Data File for QuickLink

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

Pick Method for QuickLink

Lists the eight most recently used Methods in order of use. When you select one, the Method displayed in the QuickLink button changes to the selected file.

Help On

Displays all applications on the Workstation Toolbar.

Product Support Web Site

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

About Workstation Toolbar

Displays the About box for the Workstation Toolbar, which contains information about the MS Workstation software version, installation history, and a list of the instrument control modules installed. The following is an example.

WS Workstation (Demo) (V6.9.1.B	4 05/04/07)	
Varian MS Workstation	VARIAN	
Workstation Toolbar	Version 6.9. (Service Pack 1)	
Copyright © 1989-2007, Varian, Inc.	Service Code:	
Installed Module Drivers 800 Interface Box ADC Board 8200 AutoSampler 3800 GC 3900 GC	<	and a first the second second
Installation History MS Workstation S/N: Installed by Organization: Installation date:	*	and and a second s
Validate Installed Files	Close	

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

✓ Validation of installed file systems	
File Options Help	
FILE SYSTEM VALIDATION REPORT	
File System: Varian Workstation 6.8 Workstation: ENG7665	
Directory: C:\varianws	
Source file: c:\varianws\star.val	
Test Results: 163 files tested 163 files OK *** File System OK ***	
Installation History:	
======================================	
======================================	
======================================	
======================================	
======================================	
======================================	
======================================	

Quit

Click to close the Workstation Toolbar application. If you choose to run the Workstation Toolbar automatically when Windows starts, the Workstation Toolbar reappears the next time you start Windows.

Launching Applications from the Workstation Toolbar

Application Icons



MS Workstation applications are icons on the Workstation Toolbar. As you move the cursor over them, the name of the application appears below the cursor.

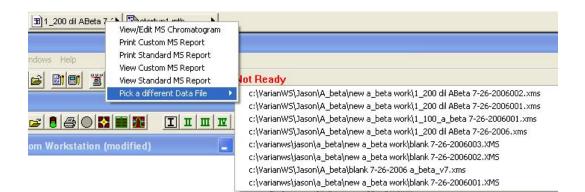
Click an icon to launch that application.

Data File and Method QuickLink Buttons



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

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



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

	View/Edit Method Print Method	
	Pick a different Method 🕨	C:\VarianWS\startup1.mth
RCL SHP	to II Not Rez	C:\VarianWS\Jason\A_beta\a_beta_v7.mth C:\VarianWS\Jason\A_beta\a_beta_v6.mth C:\VarianWS\Jason\A_beta\a_beta_v5.mth
dified)		C:\VarianWS\Jason\A_beta\a_beta_v4.mth C:\VarianWS\Jason\A_beta\a_beta_v3.mth C:\VarianWS\Jason\A_beta\a_beta_v2.mth C:\VarianWS\Jason\A_beta\a_beta_v1.mth

System Control

Overview

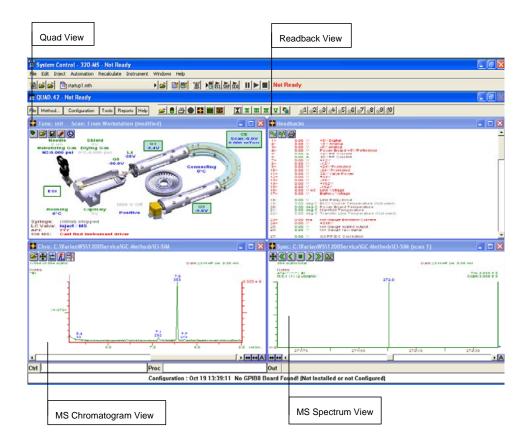
This section presents an overview of System Control functions. Other functions are explained in detail in later sections.

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

🗑 System Control - Configuration	
File Edit Inject Automation Recalculate Instrument Windows Help	
1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	
Instrument 1: MS	
Operator: Vivian Rogers	
Waiting for Instrument Modules	
AutoStart Module	
J 42	
Instrument 1 Parameters	
Available	
Modules	

Instrument Window

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



File	Edit	Inject	Automation	Recalculate
A	ctivate	e Methoo	l	
U	pload	Active M	ethod from Ma	dules
N	ew Sa	mpleList.		
0	pen Sa	ampleLis	t	
N	ew Re	calcList.	N	
0	pen R	ecalcList		
N	ew Se	quenceL	ist	
0	pen Se	equence	List	
Pi	rint			
P	rinter S	Setup		
🗸 R	ememl	oer Last	Open Files	
E	×it			
-				

System Control File Menu

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

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

New SampleList - Create a SampleList.

Open SampleList - Open an existing SampleList.

	Sample Name	Sample Ty	ре	Cal. level	lnj.	Injection Notes	AutoLink	Inj. Mode		lnj. Volume	Plate	Well / Vial	v.	Add
1	Sample 1	Analysis	-		1	none	none	Partial Loopfill	+	10.0		A1		Insert
2	Sample 2	Analysis	-		1	none	none	Partial Loopfill	-	10.0		A2		Inseit
3	Sample 3	Analysis	-		1	none	none	Partial Loopfill	-	10.0		A3		Delete
4	Sample 4	Analysis	-		1	none	none	Partial Loopfill	-	10.0		A4		Fill Dowr
5			-						-					

New RecalcList - Create a recalculation list.

Open RecalcList - Select an existing recalculation list.

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

New SequenceList - Create a sequence list.

Open SequenceList - Select an existing sequence list.

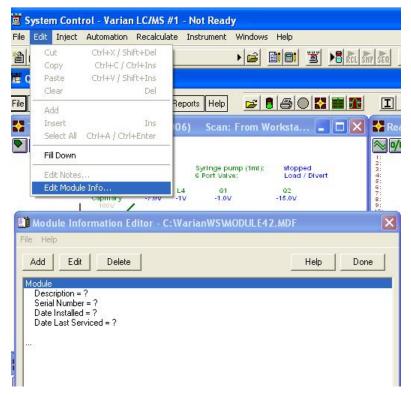
	Action		Method	Sample/RecalcList	_	
1	Inject	-	c:\varianws\minimum.mth	c:\varianws\my samplelist.smp		Add
2	Inject	-	c:\varianwsservice\gc-methods	c:\varianws\test.smp		Insert
3		-				Delete
4		-				Delete
5						
6		-				
7		-				

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

Edit Menu

Edit Module Info

Click Edit and select Edit Module Info

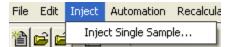


Documenting Module Information - Each module in your system (300 Series, 3800 GC, LC modules, Combi PAL, or HTS PAL AutoSampler) has a message log and screen. Use Module Information to keep a record of module

performance, maintenance, hours used, or other comments. From the System Control menu bar, select **Edit > Edit Module Info.**

Inject Single Sample Menu

Click **Inject Single Sample** to open the Inject Single Sample window. Enter information about your sample. The 300 Series Module and all modules in the system must be in the Ready state before you make an injection. You can do a manual injection or use the autosampler.



Sample Name	Sample Type	Cal. level	lnj.	Injection Notes	AutoLink	Inj. Mode		Inj. Volume	Plate	Well / Vial	Wash Volume	Automix Routines	User Program	Amount Std (IS, N% only)	Unid Pe Factor
efault Sample	Analysis 👻		1	none	none	Partial Loopfill	-	10.0		A1	300	none	2	1	0
Inight the Complex usi	a the Method														
Inject the Sample usi	ng the Method:														
	-			Browse	Defaults										
C:\VarianWS\startup	- j1.mth			Browse	Defaults										
Inject the Sample usin C:WarianWS\startup Clear Coefficients	- j1.mth			Browse	Defaults										
C:\VarianWS\startur	- j1.mth			Browse	Defaults										
C:\VarianWS\startup	- j1.mth			Browse	Defaults										

Select a Sample Type from the list:

Sample T	уре
Analysis	
Analysis	
Calibration	
Verification	
Baseline	

Click Injection Notes to enter a description or comment.

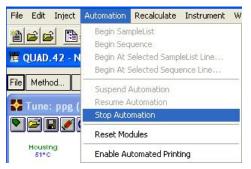
	Notes 🛛 🔀
Injection Notes	I
none	
	OK Revert Cancel

Use **AutoLink** to enter a command to execute a program after the data file is acquired. For example, you can create and print 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:\VarianWS\EPA525.swt) in the Command line. Note that Custom MS Reports templates are stored in the VarianWS directory. Use the browse command to select the command executable files.

AutoLink	AutoLink Parameters	
none	Command	Other parameters
a Defaults	Browse	OK Cancel

Make a selection and click OK.

Automation Menu



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

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

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

Suspend Automation - Stop automation after the last completed sample.

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

Stop Automation - Stop automation immediately and reset all modules.

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

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

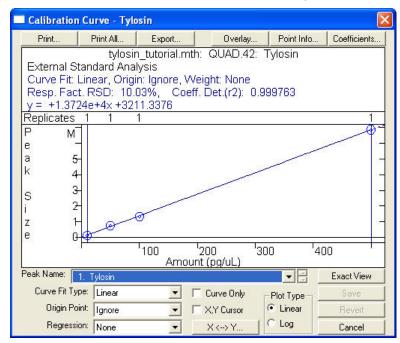
Recalculate Menu



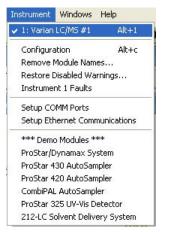
Begin RecalcList - Start an automated Recalculation. A Recalculation list must be opened under the File menu.

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

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



Instrument Menu



Varian LC/MS #1 - Configured instrument.

Configuration - Add new modules to the existing instrument, such as, a Combi PAL AutoSampler or LC pumps.

Remove Module Names - Remove associations between Module Names and Module Addresses. You can connect a Module with a different Module Name at that address. The next time the associated Module connects at that address, you are prompted to select the correct name for the Module.

Instrument 1 Faults - Determine if there are faults in any module of Instrument 1. See the following example. Click **Update** to check for new faults.

Module - Address Faults	
Module 212.24: 2 Fault(s) Module 430.33: 0 Fault(s) Module QUAD.42: 0 Fault(s)	
 Recent Messages and Faults 	Update
 Recent Messages and Faults SelfTest Messages and Faults 	Update View

Setup Ethernet Communication - Set up communication between the 3800 GC or other Ethernet modules and System Control. Refer to the Ethernet Communication Setup section in one of the following manuals for more information: Data Acquisition with 3800 GC Control (part number 391473100) or Data Acquisition with LC Control (part number 91473200).

Setup COMM Ports - Set up communication between System Control and modules communicating with the Workstation through the Serial ports on the PC. The first time you start System Control, the Star Communication Configuration Wizard starts automatically. Refer to Data Acquisition with LC Control (part number 0391473200) for more information.

Windows Menu

Windows	Help
Show M	Iodule Windows
Iconize	Module Windows
Show A	utomation Windows
Iconize	Automation Windows
Arrange	e Icons
Instrum	ent 1 Status
Messag	je Log
212.24	- Stopped
430.33	- Ready
QUAD.	42 - Not Ready

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

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

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

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

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

SequenceList - Display the active SequenceList.

SampleList - Display the active SampleList.

RecalcList - Display the active RecalcList.

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

Message Log - Tracks errors that occur during automation. Double-click the Status bar at the bottom of the Instrument window to view the message Log for all modules configured in the Instrument.

<u>^</u>

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

212.24 - Stopped

430.33 - Ready

Quad.42 - Not Ready

Help Menu

lp Topics
oduct Support Web Site
out System Control

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

Click a book, and then click Open. Or click another tab, such as Index.	lp Topics: MS Wor		control	<u> </u>
 System Control Menus System Control Toolbar System Control Windows and Dialog boxes 2000 MS Module Control 4000 MS Instrument Window 500-MS Instrument Control Quad MS Module Control (1200/1200L/310-MS/320-MS) 3400/3600 GC System Control Window 3400/3600 GC Injecting a Single Sample 3400/3600 GC System Control Command Reference 3800 GC System Control Window 3800 GC Injecting a Single Sample 3800 GC Injecting Multiple Samples 3800 GC Injecting Multiple Samples 3800 GC System Control Official Command Reference 	ontents Index Find			
 System Control Menus System Control Toolbar System Control Windows and Dialog boxes 2000 MS Module Control 4000 MS Instrument Window 500-MS Instrument Control Quad MS Module Control (1200/1200L/310-MS/320-MS) 3400/3600 GC System Control Window 3400/3600 GC Injecting a Single Sample 3400/3600 GC System Control Command Reference 3800 GC System Control Window 3800 GC Injecting a Single Sample 3800 GC Injecting Multiple Samples 3800 GC Injecting Multiple Samples 3800 GC System Control Official Command Reference 	or i i i i i	r 1 0 0 r 1		1.5
 System Control Toolbar System Control Windows and Dialog boxes 2000 MS Module Control 4000 MS Instrument Window 500-MS Instrument Control Guad MS Module Control (1200/1200L/310-MS/320-MS) 3400/3600 GC System Control Window 3400/3600 GC Injecting a Single Sample 3400/3600 GC System Control Command Reference 3800 GC Injecting a Single Sample 3800 GC Injecting Multiple Samples 3800 GC Injecting Multiple Samples 3800 GC Injecting Multiple Samples 3800 GC Injecting Control Window 3800 GC Injecting Multiple Samples 3800 GC System Control Command Reference 	LICK a DOOK, and then	Click Upen. Uf click	another (ab, such as Inc	Jex.
 System Control Windows and Dialog boxes 2000 MS Module Control 4000 MS Instrument Window 500-MS Instrument Control Guad MS Module Control (1200/1200L/310-MS/320-MS) 3400/3600 GC System Control Window 3400/3600 GC Injecting a Single Sample 3400/3600 GC System Control Command Reference 3800 GC System Control Window 3800 GC Injecting a Single Sample 3800 GC Injecting Multiple Samples 3800 GC Injecting Multiple Samples 3800 GC Injecting Multiple Samples 3800 GC System Control Window 3800 GC Injecting Multiple Samples 3800 GC System Control Command Reference 	System Control N	Menus		~
 2000 MS Module Control 4000 MS Instrument Window 500-MS Instrument Control Guad MS Module Control (1200/1200L/310-MS/320-MS) 3400/3600 GC System Control Window 3400/3600 GC Injecting a Single Sample 3400/3600 GC System Control Command Reference 3600 GC System Control Window 3800 GC Injecting a Single Sample 3800 GC Injecting Multiple Samples 3800 GC Injecting Multiple Samples 3800 GC Injecting Multiple Samples 3800 GC System Control Command Reference 	System Control 1	oolbar		
 4000 MS Instrument Window 500-MS Instrument Control Guad MS Module Control (1200/1200L/310-MS/320-MS) 3400/3600 GC System Control Window 3400/3600 GC Injecting a Single Sample 3400/3600 GC System Control Command Reference 3800 GC System Control Window 3800 GC Injecting a Single Sample 3800 GC Injecting Multiple Samples 3800 GC System Control Official Samples 3800 GC System Control Command Reference 	📚 System Control V	Vindows and Dialog	ooxes	
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3800 GC System Control Window 3800 GC Injecting a Single Sample 3800 GC Injecting Multiple Samples 3800 GC System Control Command Reference	📚 3400/3600 GC In	jecting Multiple Sampl	les	
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3800 GC Injecting Multiple Samples 3800 GC System Control Command Reference				
S800 GC System Control Command Reference	📚 3800 GC Injectinj	g a Single Sample		
	S800 GC System	Control Command Re	eference	~
		Oper	n Print	Cance

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

Help Topics: MS Workstation System Control	? 🔀
Contents Index Find	
1 Type the first few letters of the word you're looking for.	
2 Click the index entry you want, and then click Display.	
3800 GC Status and Control Window: 3800 Setup dialog box 39XL Operation Display 39XL Setup Dialog Box 4000 MS Icon 4900 Channel Display 4900 More Status Dialog Box 4900 Run Status 6200 AutoSampler 8200 AutoSampler 8400/8410 Carrousel Display 8400/8410 SampleList Window Extensions 9100 SampleList Window Extensions 9200 Prospekt Status and Control Window Acquisition Mode Active Sample Status	
Display Print	Cancel

Enter a key word or phrase to list help topics.

quad	Clear
Select some matching words to narrow your search	Options
quad Quad	Find Similar
quadrupole Quadrupole quadrupoles	Find Now
quaurupoies	Rebuild
Click a topic, then click Display AutoTune Options GC/MS Tuning El and Cl	

About System Control provides information on the MS Workstation software version, a list of the Installed Modules, and the Workstation Installation History.

Validate Installed Files tests the installed system files and documents errors using checksums produced at the factory. These reports can be printed.

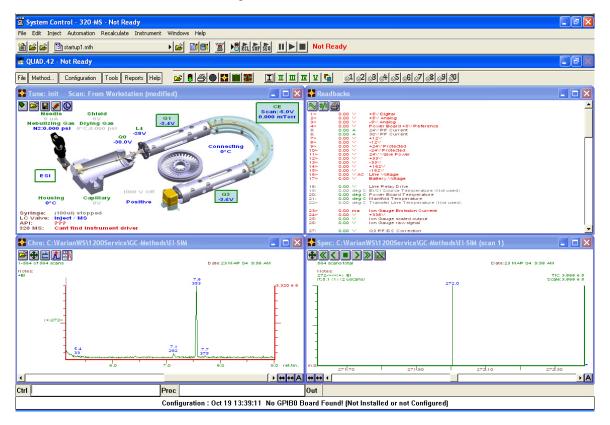
System Control Toolbar

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

🖀 🚘 🖻 startup)1.mth	• 🖻		j 😼	RCL SHP SEQ	
Create a ne	ew automation file.					
Eirst - open	an existing automa	tion file.				
Second - op	pen the Message Lo	og file.				
🗈 startup1.mth	View, edit, print	t, or reactiv	vate a m	nethod.		
Open a me	thod.					
Edit notes f	or an automation file	Э.				
Edit module	e information for any	online mo	odule.			
Display the Instrument Status	e Instrument Status Window, you can a	window w ccess mo	hen it is dule win	hidden dows if	. From the they are I	e hidden.
Inject a sing	gle sample.					
RCL Start an ac	tive RecalcList.					
Start an ac	tive SampleList.					
Start an ac	tive SequenceList.					
Suspend A	utomation.					
Begin acqu	isition.					
Stop an aut	omation run.					

Quad Status and Control Window

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



Quadrupole Module Menu

File - Open or print a file.

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

Configuration - Synchronization signal settings and MS Options settings.

E QUAD.4	2 Mat Da	and an
A UUAU.4	Z - NUL RE	auy

File	Method	Configuration	Tool
-	Tune: ppg	Sync signals.	
	28.	Options	

Start Out Signal Enabled Wiring When the instrument starts an acquisition, it closes the contact between pins 4 and 5 on Row 2, Column C of the IO connector for 500 msec.	Ready Out Signal Enabled Wiring 4 and 5 on Row 1, Column C of the ID connecter when it is ready to acquire data, and reverses it when it is not ready.
Ready In Signal Enabled Wiring The instrument senses the readiness of another device through Pins 2 and 3 at Row 2, Column A of the 10 Connector. When the state between these pins is sensed (open or closed depending upon which radio button is selected), the device is considered ready. Contact open = ready Contact closed = ready	Start In Signal Varian GC Cable 03-937179-01 GC/QuadMS Image: Constraint of the life

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

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

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

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

1	Mass-spec connection:	Automatic	Edit
1	System id :	211105154955	Edit
Currei	nt hardware configuration —		-
1.	MS Model:	320(GCLC)	Override
1.	System type:	MS/MS system (Triple quad)	Override
1.	Mass range:	8 to 2000 amu	Override
1.	Ion source type:	API Ion source	Override
Currei	nt software settings		
1	Scan Optimization:	Standard LC	Edit
1.	MS ready:	Enabled	Edit
	Pressure units:	Torr and PSI	Edit
1.	Font type:	Arial	Edit
	Print mode:	Color	Edit

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

Tools	Reports Help
Quit	: Macros
Use	r pml
Pml	Editor
Plot	tic,readbacks,
Ana	log output of
MSN	15 Breakdown
Bak	eout system
Ove	rnight Standby
Trou	ubleshooting
Inst	setup/others

Quit Macros: Stop any MS function in progress.

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

User PML	s 🛛 🛛
_ Select a P	ML
User 1	fm 10
User 2	fm 20
User 3	
User 4	
User 5	
User 6	
User 7	
User 8	
User 9	
User 10	
Apply	OK Cancel

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

6	1)_2	୍ଷ	Ħ	୍ଦ୍ୟ	୍ତେ	7	ୖଃ	୍ର	10
Ì	User F	ML 1	: fm	10					

Plot tic, readbacks - Plot a graph of the TIC, up to 2 masses, up to 2 readbacks, or a PML to monitor instrument status. Check In use and the check box next to the desired parameter and then click Apply.

Plot in pict view		X
🔲 In use	Clear Pict View	
🗔 тіс		
Area of mass	100.0	
Area of mass	200.0	
🔲 Readback	1: +5V Digital	•
🔲 Readback	1: +5V Digital 2: +5V Analog	^
F PML	3: -5V Analog 4: Power Board +5V Reference 5: +24V RF Current 6: -24V RF Current	~
	Apply Exit	

Analog output - For service use only.

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

Bakeout System

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

Overnight Standby - Turns off all gases and sets the MS to a low scan mass.

MS Standby	
Put MS into standby now	Put MS into standby while idle ✓ Enable auto-standby The MS is idle if the sysem is not on and there is no keyboard input or data collection happening. After the system is idle for the given number of minutes, the system
[will go into standby and execute the following PML 60 Minutes OK Cancel

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

Inst setup/others - Perform initial instrument setup operations.

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

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

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

Reports - Select a print view setup.

Help - Online Help and the About window.

Reports - Select a print view setup.

Help - Online Help and the About window.

Quadrupole Toolbar



Choose File to Display - Open and delete data files, and edit headers.

Start Collecting Data - Acquire data from only the 300 Series and not other configured modules. Collect the current scan, which may not be the active method.

File name:	APR 11 2007 12	2-14	
	Browse	File naming methods	
Operator:			
Sample Id:	Default Sample		
Notes:			
	6	.dd [[5.0 min. to ru	



Print - Print the window screen.

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

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

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

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

EI/CI Source Analyzer	(),C •	
Calibration Gas	Filament Current ○ On ○ Off ▼ In Use 150 uA (50 to 500) Typical: 50	Discharge C On C Off [In Use 1500 to 2000) Typicat 1500
Electron Energy	€ 70 eV	150 eV
Source Temperation	and a second	Actual 0 °C
Transfer Line Ten Requested 0	deg C (10 to 400)	Actual 0 °C
Apply	ОК	Cancel

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

istrument Parameters	
APISource Analyzer Safety Syringe Pump	
API Analyzer voltages on I lonization mode API on-off sequence	
C APCI C Manual	
N2 Filling Time 10 Sec. Equilibration time 10 Sec.	
Gases ↓ Drying gas 18.0 psi	
₩ Nebulizing gas 55.0 psi	
Vaporizer gas 18.0 psi	
Nebulizing gas type	
Heaters	
✓ API Housing (0-65) 50 actual 50 °C (18% on)	
Drying gas (50-400) 200 actual 199 °C (21% on)	
Vaporizer gas (50-550) 550 actual 600 °C (0% on)	
Apply OK Cancel	

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

Pumps	CID gas	- Manifol	d
High Vacuum	⊙ On	42	Deg. C
Vent	C Off CID gas pressure	2300) to 65) bical: 40
Turbo Speed	2.00 mT orr	Manifold	temperature
99 %	2.00 mTorr	4:	2 Deg
Detector (600 · 2000	Volts)		
Off Extended Dyr		tem	ernal Air perature 3 Deg
Fixed	1500 Volts	Manifo	ld Pressure
Optimize		1.3	e-5 Torr
Detector optimum = 1	890 Volts		
Detector calibration is 30 days	recommended every		
Detector gain last cor	mputed Apr 10,2007		

Safety - has three sections. Only Varian Representatives can make changes.

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

strument Pa	rameters	ŧ	
NPI Source An	alyzer Sal	fety Syringe Pump	
PCB Prote			Trip Points
		m is in automatic mode. m is in manual mode.	Source Pressure:
L HA E	nable –	lon Gauge-	Manifold Pressure:
0	Auto	C Auto	1.00 mTorr
	On	C On	Turbo Speed :
C	Off	COH	90 % full speed
	Apply	οκ	Cancel

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

nstrument	Parameters
API Source	Analyzer Safety Syringe Pump
Syringe	e pump status: Stopped
s	tart Purge Stop
Infusi	
Spe	
	e cycle
Spe	ed 7.89 ul/Min. (0.01 to 7.89)
Syrin	ge type Brand Volume
	Standard size Hamilton
	Add/Delete syringe to/from Standard size list
	Brand Volume Diameter
	mm ID
	Save Syringe Delete Syringe
	Save Synnige Delete Synnige
C	Other 0.46 mm ID
	,
	Apply OK Cancel

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

12. 13.	
Method Specs.	Time segment 1 of 1
Model 320(GC&LC) 🔽	Add seg Remove seg Start at retention 0.00 Min.
Ionization ESI	Scan Time (in Seconds) If Collect Data If CID gas on Requested Time 0.000 Mass peak width in amu Used Scan Time: 0.000 Quad 1 Calibrated
Data type	Mass List
Centroid	Add Insert Delete Clear All Cut Copy Paste Fill Down FD and I
Collect delay	Polarity Q1 First Q1 Last Q3 First Q3 Last Mass Mass Mass Capillary Collision Req. Dwell Act. Dwell Act. Dwell
🔽 Use delay	1 Pos. 219.00 50.00 300.00 5.000 0.120 0.166

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

AutoTune Tune and Calibrate Calibrate Report Tune to target ratios Calibrate detector (EDR) Stop tuning Standard Compound(s) End Label Add high mass tune points Use fixed detector value in	 Don'	A contraction of the formula of the
, Add high mass tune points Use fixed detector value in Comments:	report	

300 Series Module Views

🗱 QUAD.42 - Not Ready							
File 1	Method	Configuration	Tools	Reports Help	2 8608 2 6	I I I I V V 🖬)

The five default views are:

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

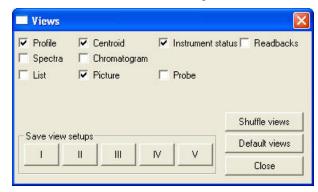
View II - Displays Quad Instrument status, Chromatogram, Spectra, and Centroid windows.

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

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

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

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



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

Spectra - Post acquisition display of either profile or centroid spectra from the chromatograms.

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

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

Chromatogram - Real time or post acquisition display of chromatograms.

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

Instrument Status - Graphic of the analyzer, showing temperature and pressure status.

Readbacks - Real time text display of either analog or digital instrument parameters.

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

300 Series Autotune Functions and Options

NOTE: For a detailed description of Autotune steps, refer to the LC/MS and GC/MS sections in the 300 Series Hardware Operation Manual.

Overview

Autotune optimizes the instrument for sensitivity, resolution, and mass calibration.

For LC/MS, a reference compound such as polypropylene glycol (PPG) is used as a tuning solution. You may also use a custom tuning solution.

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

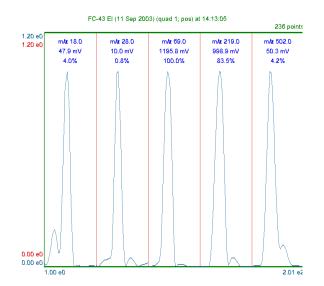
Both quadrupoles can be tuned in both polarities (positive and negative). A report with a display of the peak shapes and intensities and a text report with tuning details is displayed and saved to c:\varianws\methods directory. See the following.

Tune report for Varian 1200

Time: 14:13:05 Tune file: FC-43 EI (11 Sep 2003)

mass (amu) 18.0	mass	Mass	Peak	Relative	Peak	Valley	Resolution
		error	height	height	width		
10 0	(amu)	(amu)	(mV)	(%)	(amu @ 50%)	(% of iso)	(m/delta-m)
10.0	18.2	0.2	47.9	4.0	0.58	100	32
28.0	28.1	0.1	10.0	0.8	0.55	100	52
69.0	69.0	0.0	1195.8	100.0	0.69	100	101
219.0	219.0	-0.0	998.9	83.5	0.75	79	290
502.0	501.9	-0.0	50.3	4.2	0.68	18	741
etector =	1440 V)						
•	for Varian						
•	for Varian 07 Tune fi		EI (11 Se	ep 2003)			
•	07 Tune fi		EI (11 Se Peak	ep 2003) Relative	Peak	Valley	Resolution
- me: 14:16:	07 Tune fi	le: FC-43	Peak	•	Peak width	Valley	Resolution
- me: 14:16: Exact	07 Tune fi Measured mass	le: FC-43 Mass	Peak	Relative height			Resolution (m/delta-m)
ne: 14:16: Exact mass	07 Tune fi Measured mass	le: FC-43 Mass error (amu)	Peak height	Relative height (%)	width		
ne: 14:16: Exact mass (amu)	07 Tune fi Measured mass (amu) 18.2	le: FC-43 Mass error (amu) 0.2	Peak height (mV) 593.5	Relative height (%)	width (amu @ 50%)	(% of iso)	(m/delta-m)
- me: 14:16: Exact mass (amu) 18.0 28.0	07 Tune fi Measured mass (amu) 18.2	le: FC-43 Mass error (amu) 0.2 0.1	Peak height (mV) 593.5	Relative height (%) 38.7 10.6	width (amu @ 50%) 0.54	(% of iso) 100	(m/delta-m) 34
.me: 14:16: Exact mass (amu) 18.0 28.0 69.0	07 Tune fi Measured mass (amu) 18.2 28.1	le: FC-43 Mass error (amu) 0.2 0.1 -0.0	Peak height (mV) 593.5 162.6 1535.2	Relative height (%) 38.7 10.6	width (amu @ 50%) 0.54 0.62	(% of iso) 100 100 100	(m/delta-m) 34 45

Tuning of quad 3 in positive mode successfully completed.



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

The tuning compound signal must be stable before starting the Autotune procedure (Cal Gas on for at least 10 minutes, and signal from PPG infusion stable).

NOTE: It is not necessary to tune the instrument daily. Tune if the ion source becomes contaminated and there is a significant loss of signal. If this happens, clean the ion source and AutoTune.

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

AutoTune Options

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

AutoTune		
Tune and Calibrate Calibrate Report Tune to target ratios	Analyzer C Quad 1 C Quad 3 C Both	Polarity C Positive C Negative C Both
Calibrate detector (EDR)	C Single from list	+59.000
Standard Compound(s)	Ec	lit Standard Compound(s)
PPg	F	actory compound
🔲 Add high mass tune poir	nts 🔽 Don't I	turn on Calibration Gas
🔲 Use fixed detector value	in report	
Comments:	ve and negative tuning,	over the entire mass range.
		Cancel

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

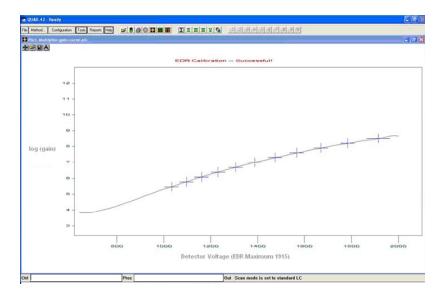
A report is generated with a graphic of the peak shapes and intensities (saved with mode name and date) and a text report with detailed mass accuracy and mass abundance.

Calibrate - Update the loaded tune file by re-tuning mass resolution and recalibrating the mass. No changes are made to settings in the ion source or the non-analyzing quadrupoles. A new file name and report are created and saved. **Report -** Create and save a tune report. Verify tune stability by comparing with previous reports to determine if re-tuning is required. Creating a report does not change the tune file.

Tune to Target Ratios - Modify existing tune files. See 'Tune to Target Ion Ratios' Section.

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

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



The plot shows detector gain as a function of detector voltage.

Stop Tuning - Abort the Tuning procedures and restores the most recent Tune file.

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

Polarity - Set AutoTune polarity mode.

GC/MS

- CI AutoTune either positive or negative
- EI AutoTune positive only

LC/MS

ESI - AutoTune either positive or negative (for APCI use ESI tune file)

lon(s) - Select either a specific ion or all defined ions in the Compound list. If you choose Single from the list, select an ion from a list of ions in the Standard compound. Using a single ion adds a new data point to the loaded tune file and

does not change existing points. If the same mass is already present, it is tuned and changed accordingly. A report for this single mass is created and the tune file is named and saved.

Edit Standard Compound(s) - Open Compound Editor. You can modify a Standard compound or create a list of new compounds.

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

Cancel - Close the Autotune window without executing a function.

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

Compound Name/Mode (Date created).dac

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

Example: Second Negative CI Tuning on October 6th 2003

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

Tune to Target Ratios

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

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

Click either Tune the Calibration Gas Ratios directly, or Use a previously acquired data file.

To tune the calibration gas ratios directly:

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

Tune and Calibrate	Analyzer C Quad 1	Polarity Positive
Calibrate	C Quad 3	C Negative
Report	Both Both Construction Second S	C Both
Tune to target ratios	lon(s)	-
Calibrate detector (EDR)	○ Single from list	+18.000 -
Stop tuning	All	
tandard Compound(s)	Edit	Standard Compound(s)
FC-43 EI	▼ Fac	ctory compound
Add high mass tune poin	ts 🗌 🗌 Don't tu	n on Calibration Gas
Use fixed detector value	in report	1
Comments:		
For positive EI tuning only.		

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

Tune to targ	get ratios 🛛 🔀
Tune Ca	libration Gas Ratios directly
Use a previous	y acquired data file (DFTPP, etc.)
	Cancel

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

Input the target ion r	atios (or restore from file)
Mass	% Area
69.0	100.0
131.0	55.0
219.0	50.0
414.0	2.0
502.0	2.0
Save R	estore Close

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

Varian Quadrupole Mass Spec
Mass 69, target: 100.0-100.0%, measured 100.0%. Needs reduction: 48.1% Mass 131, target: 94.0-96.0%, measured 49.0%. Needs reduction: 0.0% Mass 219, target: 49.0-51.0%, measured 76.7%. Needs reduction: 65.8% (Too much)!!! Mass 414, target: 1.0-3.0%, measured 6.5%. Needs reduction: 80.0% (Too much)!!! Mass 502, target: 1.0-3.0%, measured 7.2%. Needs reduction: 82.0% (Too much)!!! If calibration gas ratios need too much adjustment, you may want to consider first - Checking air/water levels - Autotune - Cleaning the ion source
OK to proceed?
OK Cancel

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

Standard Compound Editor

GC/MS EI Example

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

Standard Compounds				
Standard Compound:				Remove
FC-43 El 💽 Factory con	pound	🔲 Default for thi	s mode	New
Comments:				(New
For positive EI tuning only. Ion Source				
Positive Ions	Negative	lons		
Use in Use in Exact No. of Tune Report m/z isotopes		Use in Exact Report m/z	No. of isotopes	8
M 18.000 1				
R 28.006 1			ī Ē	

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

Define new standa	rd compound	
Please enter a name	e for the new stand	lard compound:
My Standard Compou	nd	
🔽 Clear all fields	ОК	Cancel

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

Standa	rd Comp	ounds							
Standard	d Compour	nd:							Remove
My Stan	dard Comp	oound	💌 U	lser defined cor	mpound	☐ Def	ault for this	mode	New
Commen	its:								14000
1									
Ion Sour	rce 🔳	-	-						
Positive	lons				Negativ	e lons			
Use in Tune	Use in Report	Exact m/z	No. of isotopes		Use in Tune	Use in Report	Exact m/z	No. of	
	Г	11/2					111/2	isotopes	
F	Г	-	-		Г	Г	-	-	
Ē	Г	-	-		Г	Г	-	-	
Г	Г	-	-		Г	Г	-	-	
Ē	Г	-	-		Г	Г	-	-	
Ē	Ē	-	-		-	Г	-	-	
-	Г	-	-		_	_			
-	Г	-			-	, _	<u> </u>		
-	-	-				, 	<u> </u>		
-	-		L		- -	Г			
	1					1			
							Apply	OK	Cancel
								-	

Standard Compound - List Standard Compounds for the selected mode.

Default for this Mode - Set displayed Standard Compound as the default for the selected mode.

New - Add new list of Standard Compounds.

Remove - Remove a Standard Compound.

Comments - Enter information about the Standard Compound.

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

Use in Tune - Select which ions are used for Tune or Calibrate. The selected ions are optimized.

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

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

No. of Isotopes - Enter the number of isotopes for the ion displayed in the tune report graphic.

LC/MS ESI Example

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

PPg	d Compour	nd:	-	Factory com	oound	🔽 Def	ault for this i	mode	Remove
Commen									11011
	sed for bo ass range.	th positive a	nd negativ	e tuning, over l	he				
	_		-						
Ion Sour	ce <mark>ES</mark>	<u>-</u>	া দিঃ	Set Capillary					
Positive	lons				Negativ	e lons			
Use in Tune	Use in Report	Exact m/z	No. of isotopes	Capillary (Volts)	Use in Tune	Use in Report	Exact m/z	No. of isotopes	Capillary (Volts)
ম	ম	59.000	1	100.00	जा	Tepol(45.000	1	-40.00
1	2	175.100	1	100.00	ম	V	469.300	2	-40.00
V	V	442.300	2	30.00	ম	5	817.600	3	-60.00
V	V	790.600	3	80.00	ম	5	1049.70	3	-80.00
V	ম	1138.80	3	100.00		Г			
Г							-		
Г	Г	<u> </u>	<u>_</u>	<u> </u>		Г	-	-	
Г		<u> </u>		<u> </u>			-	-	
Г		<u> </u>					-	-	
Г	Г	<u> </u>		·	Г	Г	-		
		1		1			1	1	1

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

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

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

300 Series Method Builder

Quad Method Builder

Click Method Builder in the MS WorkStation Toolbar.



Edit an Existing Method

Sometimes it is easier to modify an existing method than building a new method.

1. Select **Open** an Existing Method File and click **OK**.

Create/Open Method File	
Select a method file action C Create a New Method File C Open an Existing Method File	OK Cancel
Do not display this dialog at startup	

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

Open Metho	d File	? 🛛
Look in: 🔀	ChromExamples 🗾 🗲 🔁	r 📰 🕈
ANOTHER.	ITH Iminimum.mth Imve.mth Mth Imve_exame.mth ITH Imparade.mth I Imparais.mth	
File name:		Open
Files of type:	Methods (".mth)	Cancel Recent Files >

• Click Recent Files to display them and select one.

1		
	Open Method File	<u>? ×</u>
ĺ	Look in: 🗀 ChromExamples 💽 🗲 🖆 🗄	-
	Image: Second	
	File name:	Open
	Files of type: Methods (".mth)	Cancel
	Rec	C:\VarianWS\ChromExamples\IDENT.MTH C:\VarianWS\ChromExamples\ES_EXAMP.MTH C:\VarianWS\ChromExamples\PEXAMP.MTH C:\VarianWS\ChromExamples\parais.mth C:\VarianWS\ChromExamples\VP_EXAMP.MTH C:\VarianWS\ChromExamples\VP_EXAMP.MTH C:\VarianWS\ChromExamples\NT_STD.MTH C:\VarianWS\ChromExamples\ANOTHER.MTH C:\VarianWS\ChromExamples\SUBTRACT.MTH

Build a New Method with the Configured Instrument

- 1. Select Create a New Method File and click OK to open the Method Builder Wizard.
- 2. Select **Instrument 1**. The configured instrument is added to the method.

3. Click Next.

Select Configuration		×
	Select an existing instrument configuration for the method or select a custom configuration for the method. Then click Next to continue. Select a Configuration Custom Instrument 1 Configuration Description Module Address 212 3 Custom QUAD 42	
	< Back Next > Cancel	

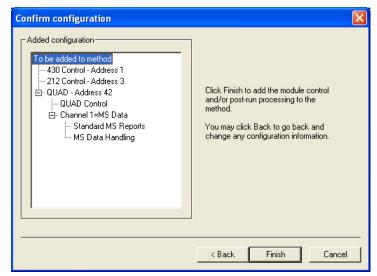
- 4. Select a detector. After the data is acquired you can add data processing information to the method.
- 5. Click Next.

Select detectors for post-run processing		
	Select the detector(s) for which you want to add post-run processing to the method. Then click Next to continue. Detector Modules VQuad Mass Spec at address 42 Unselect All	
	< Back Next > Cancel	

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

Create sections for post-run processing						
For the following module: QU	AD at address 42					
Select the channel(s) to process:	Select the Post-Run processes to perform: Interpretation of the second					
Unselect All						

- 8. Review the information on the **Confirm configuration** screen.
- 9. Click Next.
- 10. Review the configuration
 - Click **Back** to make changes
 - Click **Finish** to confirm.



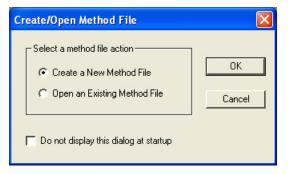
11. The new method is displayed with a navigation tree on the left side and the method workspace on the right. Click a tree entry to open that method section.

🖹 Method Builder - [Method1*]		
🖺 File Edit View Window Help		_ 8 ×
File Edit View Window Help Edit View Window Help Method Profile Edit View Window Help Method Profile Edit Method Profile Edit Profile Edit Method Profile Edit Profile Edit Profile Ed	Location: (Method File Not Saved) Created: Modified: Size: 22892 bytes Method File Attributes Bread-only Hidden Archive Requires Password on Save Revision History:	
Compound Reports Calibration Block Report Format Summary Report Format State Handling Calculations Setup Compound Table Results Treatment	(No Revision History)	
Ready		NUM //

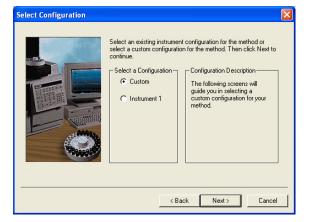
Build a New Method adding a Varian Instrument

You can build a method as follows:

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



2. Select Custom and click Next.



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

the list of configured modules for the configured modules. Click Next to c Available Modules		nove to remove a m Configured Modul	
ProStar 310 UV-Vis Detect ProStar 325 UV-Vis Detect ProStar 335 PDA Detector ProStar 335 PDA Detector ProStar 400 AutoSampler ProStar 400 AutoSampler ProStar 420 AutoSampler ProStar 420 AutoSampler ProStar 420 AutoSampler ProStar 420 AutoSampler ProStar 500 CVM ProStar 400 AutoSampler ProStar 500 CVM	Add -> Add All -> <- Remove	Address 24 • 42 • 25 •	Module 212 QUAD 430

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

300 Series Acquisition Method

Click Acquisition Method in the Method Builder tree.

Set scan segments and define MRM experiments. The Mass List has a toolbar that makes completing the table as easy as using a spreadsheet.

nization ESI	I⊽ (0.500	in Seconds	Г	D gas on Mass per Quad 1 1	k width in 0	amu	ad 3 1.0	on time 0.00	Min. Copy to al
Data type		s List vdd 1	Insert	Delete	Clear All	Cut	Copy	Paste	Fill Dowr	FD and I
Centroid	-		insen	Delete	Clear All	cut		Paste	- Fill Dowr	rb and i
C Profile Collect delay		Polarity	Q1 First Mass	Q1 Last Mass	Q3 First Mass	Q3 Last Mass	Capillary	Collision Energy	Req. Dwell	
Use delay	1	Neg.	138.00				-46.000		0.500	1
Min.	2	Pos.				-				
 Display collected 	3	Pos.							1	
	4	Pos.								
Detector	5	Pos.	1						- 3	
Use EDR	6	Pos.								
EDR Maximum	7	Pos.		_						
C 1500.0 Volt	8	Pos.								
10	9	Pos.					-			
Detector off at method end	10	Pos.								
method end	11	Pos. Pos.	1				-			
Scan width in SIM	13	Pos.								
and MRM mode	14	Pos.	-				-		1	
0.70 amu	15	Pos.								
	16	Pos.	-			-			1	
lo overrides in effect	17	Pos.								
	18	Pos.					-			

Method Specifications

The following explains the Method Specifications in the Acquisition Method.

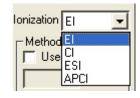
Model

Select your instrument Model.

Method Specs.			
Model 320(GC&LC			
Ionizatio — Metho	1200 1200L 300(GC) 310(LC)		
	310(LC) 320(GC&LC)		

Ionization

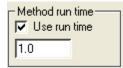
Select the ionization mode (EI, CI, ESI, APCI) - Electron Ionization, Chemical Ionization, Electrospray Ionization, or Atmospheric Pressure Chemical Ionization.



Method Run Time

You have two choices:

- Select Use run time.
- Enter a time in minutes. If you do not enter a run time, the data will be acquired until the end time is reached in all other modules.



Data Type

Set the scan type (Centroid, Profile).

Note: Quantitation can be done in ether Profile or Centroid mode.

Scan				
e	Centroid			
0	Profile			

Collect Delay

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

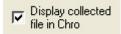
To delay data collection after the run starts, do the following:

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

Min.

Display File in Chro

Enable to display data files in Chro.



Detector

- **Use EDR** (Extended dynamic range) the detector automatically adjusts the detector voltage over the dynamic range. EDR is calibrated during the Autotune procedure (see the '*Autotune Functions*' section).
- EDR Maximum Use the optimum fixed voltage for maximum gain from the last EDR calibration (useful for low-intensity MS/MS experiments).
- Fixed Voltage Enter a fixed voltage for the entire method or different ones for each segment using Advanced Options.
- You can have the detector turn off when the method ends.

Det	ector				
	Use EDR				
C EDR Maximum					
С	1500.0	Volt			
Detector off at method end					

Scan Width

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

Scan widtł and MRM				
0.70 amu				

Time Segment

Use the arrows to select time segments. Use **Add seg** and **Remove seg** to add and remove time segments from the scan method. Start at Retention Time defines the retention time start for each segment.



Scan Time

Set the scan speed of the MS. The scan speed is the amount of time the analyzing quadrupole goes through the scan. For full scan or MS/MS scan experiments set the scan time to 0.5 seconds. The shorter the Scan Time the more data points can be acquired. Increasing the scan time increases signal to noise since the quadrupole spends more time on the particular ion. For SIM, SRM, and MRM, decreasing the scan time allows more transitions to be scanned across a chromatographic peak. When there are multiple full scan ranges in a single method segment, they must all scan at the same rate; despite the

requested dwell time. The software gives each mass range a dwell time according to the overall Scan Time and the relative sizes of each full scan range.

Scan Time (in Seconds)	
0.500	
	ī

Collision Cell Gas

Select to enable the CID gas (such as Argon) for MS/MS operations.

🔽 CID gas on

Peak Width

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

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

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

⊢ ^{Mass} p	eak width in	amu—
Quad 1	Calibrated	-
	Calibrated	~
	0.8	
e Cle	0.9	
	1.0	1
1	1.2	
Last Q	1.5	~

Mass List

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

Q3 is used for triple quadrupole instruments only.

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

Ion Polarity

Click the Ion Polarity entry to switch between positive or negative ion detection.

	Polarity	GO
1	Pos.	LC
2	Neg.	E

C/MS EI positive CI positive and negative C/MS ESI positive and negative APCI positive and negative

Capillary

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

Capillary
20.000

Collision Energy

For triple quadrupole instruments only.

The Collision Energy is experimentally determined for each reaction and entered into the Mass List. It defines collision energies in electron volts for specific MS/MS reactions used in the collision cell. (Refer to the 300 Series Hardware Operation Manual, *MS*, and *MS/MS*).



Requested Dwell Time

Specify the Requested dwell time of each scan channel. The shorter the dwell time allows more channels to be used. Specify either the scan time or the dwell time.



Mass List Toolbar

Enter values in the Mass List in a similar manner as a spreadsheet. You can Add, Insert, Delete or Clear all lines; Cut, Copy Paste from a cell or a line. You can also fill down a column, or fill down or increment the values in a column (FD and I). You can copy and paste from or to an Excel spreadsheet.



Advanced Options

Use Advanced Options to tailor your method. The Advanced Options of the 320-MS LC/GC/MS are displayed. These vary by ionization mode, instrument, and the optional ion sources (APCI and DIP/DEP probe).

The advanced options depend on the ionization mode.

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

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

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

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

El Overrides

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

Use verrides	F	Reset to defa	aults	
Г	Detector Voltage	1000	v	Copy to all
Г	Source Temperature	150	с	Copy to all
Γ	CID Gas Pressure	2.00	mTorr	Copy to all

CI Overrides

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

Use Overrides	Re	set to defa	aults	
Γ	Detector Voltage	1000	٧	Copy to al
Г	Source Temperature	150	С	Copy to al
	CI Gas Pressure	7.00	Torr	Copy to al
Γ	CID Gas Pressure	2.00	mTorr	Copy to a

ESI Overrides

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

	Time segment 1 of 1		Copy I	to all segment
Disable (l lle			
Use override	Reset	to current	values	
Г	Detector	1000	V .	Copy to all
Г	Needle Voltage Positive:	500	V	Copy to all
Γ	Needle Voltage Negative:	-500	V	Copy to all
Γ	Spray Shield Voltage Positive:	25	٧	Copy to all
Γ	Spray Shield Voltage Negative:	-25	V	Copy to all
Γ	Spray Chamber Temperature	0	С	
Г	Drying Gas Temperature	50	С	Copy to all
Γ	CID Gas Pressure	1.50	mTorr	Copy to all
Γ	Nebulizing Gas Pressure	55.0	psi	Copy to all
	Drying Gas Pressure	18.0	psi	Copy to all

APCI Overrides

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

	Time segment 1 of 1		Copy t	o all segments
Disable a	all			
Use override	Reset	to current	values	
Г	Detector	1000	V J	Copy to all
Г	Corona Current Positive:	1.00	uА	Copy to all
Г	Corona Current Negative:	-1.00	uA	Copy to all
Г	Spray Shield Voltage Positive:	25	۷	Copy to all
Γ	Spray Shield Voltage Negative:	-25	٧	Copy to all
Г	Spray Chamber Temperature	0	С	
Г	Drying Gas Temperature	50	С	Copy to all
Γ	Vaporizer Gas Temperature	50	С	Copy to all
Г	CID Gas Pressure	1.50	mTorr	Copy to all
Г	Nebulizing Gas Pressure	55.0	psi	Copy to all
Г	Drying Gas Pressure	18.0	psi	Copy to all
Г	Vaporizer Gas Pressure	18.0	psi	Copy to all

User Analog In/Outs

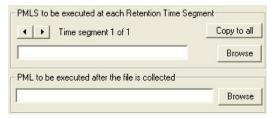
Use the Analog outputs to send the TIC signal to another device such as a LIMS system.

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

Analog output #1 (User I/O conner	ctor-> Signal = pin 14 , Gnd = pin 32 +/-5 Volts)—		
No output			
C Output TIC			
C Output TIC * 10			
C Output TIC x 100			
Output TIC x 1000			
Analog output #2 (User I/O conner	ctor-> Signal = pin 33,Gnd = pin 15 +/-5 Volts)-		
No output			
C Output TIC x 1			
C Output TIC x 10			
C Output TIC x 100			
Output TIC x 1000			
Collect User Traces			
🗂 User Input 1	Chro label:		
🔲 User Input 2	Chro label:		
F User Input 2	Chro label: Chro label:		
User Input 2 User Input 3 Readback Detector			

PMLs (Paw Macro Language)

Varian provides PML macros you can run either before or after a time segment. You can modify and create PMLs through Tools in the Quad Module View.



CI Gas Type

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

CI Gas	Туре
•	Methane
С	Isobutane
С	Ammonia
С	Other

ESI and APCI Drying Gas

Use the SelectTemp[™] feature to ensure the optimum drying gas temperature for the mobile phase composition for ESI or APCI runs.

Drying Gas L	emperature Program in	use
	Temperatures (°C)	Times (minutes)
	Initial temp	Initial Time
	200.0	0.0
Rate (°C / min)	Final temp.	Hold Time

ESI and APCI: Valve and Syringe Pump

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

Use of t	he Six-Port Valve
	Manual
	C Diverter
	C Injector
	oad position required for ready state
Syringe	Pump
	🔲 Use Syringe Pump
	Flow Rate 1.00 uL/min

APCI Vaporizer Gas

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

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

DIP/DEP Probe (Optional Ion Source)

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

Probe Type Hardware Method	Constant current	50	mA			
 Exposure probe Insertion probe Current range: 0 to 1500 mA Rate range: 2 - 2000 mA/min 	Programmed C Use Rate (mA/min) Seg 1	Initial curr (D End curr (r	j	Hold time (min)		
Standby current C Enable Standby 0 mA	Changes current ramp to Changes current ramp to Cuse Initial probe current Final probe current Maximum ramp rate			0.0 minutes al strength mA mA mA		
Quick Start Save Restore	Target ion signal strength 10.0 % full scale Ion signal type C Intensity of ions scanned © Intensity of mass 50.0 to					

Setting up MS and MS/MS Acquisitions

Overview

MS Operations

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

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

MS/MS Operations

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

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

MS Operations

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

Example:

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

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

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

Example:

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

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

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

Example:

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

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

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

Example:

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

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

Multiple Time Windows - Several time windows (Segments) can be created for an acquisition. You can do full scan, SIM, or mixed operations in each time segment and select either positive or negative polarity.

Time segmen	t 2 of 3				
	Add seg	Remove seg	Start at retention time	0.10	Min.

MS/MS Operations

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

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

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

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

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

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

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

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

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

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

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

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

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

Example:

Line 1 - Positive SIM: Precursor 452, Product 225

Line 2 - Positive SIM: Precursor 525, Product 315

Line 3 - Positive SIM: Precursor 633, Product 380

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

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

Example:

Line 1 - Positive SIM: Precursor 480, Product 225

- Line 2 Negative SIM: Precursor 612, Product 375
- Line 3 Positive SIM: Precursor 452, Product 225
- Line 4 Negative SIM: Precursor 688, Product 315

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

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

Ì	Time segmen	nt 3 of 4				
	• •	Add seg	Remove seg	Start at retention time	0.20	Min.

Injecting Samples

There are four steps in data acquisition:

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

Overview

To make a single injection, use Inject Single Sample.

To program multiple injections, use SampleList.

If System Control is not displayed, click this icon Workstation Toolbar.

Startup / Shutdown of LC/MS and Analyzer

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

Startup

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

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



Shutdown

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

320-MS LC/MS Syringe Pump and Valve

You can use the six-port valve to divert flow away from the 320-MS, or to make injections. You can also set the flow of the syringe pump and have the pump shut off at the end of the method.

Refer to the 300 Series LC/MS and GC/MS Quadrupole Hardware Operation Manual to set up the syringe pump.

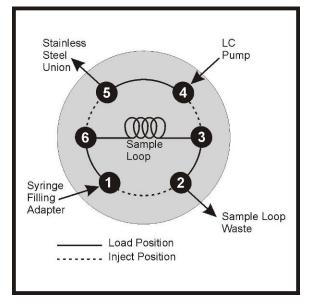
- 1. Click Advanced Options and select the Valve and Syringe Pump tab.
- 2. Select Manual, Diverter, or Diverter for the valve.
- 3. The system can turn the syringe pump off at the end of the run.
- 4. Enable the syringe pump, set the flow, and turn it off when the method is done.

venides vaiv	e and Syringe Pump Drying Gas User Analogs In/Out PMLs
	Use of the Six-Port Valve
	Manual
	C Diverter
	C Injector
	Load position required for ready state
	Syringe Pump
	🔽 Use Syringe Pump
	Flow Rate 50.00 uL/min
	Turn off at end of method

LC/MS Manual Injections

Manual Injection

Plumb the switching valve as shown.



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



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

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

Collect data	a file on c:\VarianWS\data\ APR 22 2007 12-14	× -
Operator:	Browse File naming metho	Automatic File Naming
Sample Id: Notes:	Default Sample	C Default name sample C Date and Time
Start MS	Add 5.0 min. to Stop MS Apply OK Canc	C Month Day Year and sequence no (Jan 27 1999 #001)
		Auto-increment
		Name Reserpine OK Sequence # 1 digits: 2 Cancel

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

File name:	APR 11 2007 12-14				
	Browse	File naming methods			
Operator:					
Sample Id:	Default Sample	9			
Notes:					
		con lless			
		Add 5.0 min. to run			

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

GC/MS or LC/MS Injecting Single Samples

To do one injection, either select **Inject Single Sample** from the **Inject** menu or click the **Inject Singe Sample** icon on the System Control menu bar.

File Ed	it Inj	ect	Automation	Recalculate	Instrument	Windows Help	
1	E	Injec	t Single Samp	ble		· 🛋 🛍 📾 💆	•8

If you select **Inject Single Sample** from the Inject menu, the following window opens. The fields are dependent on the sampling device.

Inject Single Samp	le									
Sample Name	Sample Type	Cal. level	lnj.	Injection Notes	AutoLink	Inj. Mode		Inj. Volume	Plate	Well / Vial
Default Sample	Analysis 👻		1	none	none	Partial Loopfill	-	10.0		A1
Inject the Sample usi	ng the Method:									
Inject the Sample usi	ng the Method:									
C. Warian WS \startu	o1.mth			Browse	Defaults					
Clear Coefficients	before Calibrating									
Inject Cano	el			Data Files.	. RecalcList					

Enter the Data File Name and Path

Data File names can up to 255 characters. You can make them a combination of Sample ID, injection date, module name, and injection number.

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

extension in the Data File name. Directory for Data Files		Data File names
🗁 c:\	^	%s %d
varianws 1200Service 1200Sys Autotune Logs BC data Beth BootlegRC10 ChromExamples data Ed_Carbamate Examples		Example: Sample 1 8-30-2006 Use the following symbols to enter th corresponding variable data to the fil name. %s = Sample ID
New Folder Drives:		%i = Injection number %d = Date %m = Detector Module name %t = Injection Time %h = Method Name %o = Operator Name %n = Instrument Name

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

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

Select a RecalcList

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

Click **RelcalcList** to open the RelcalcList Generation window. You can create a new RecalcList, append to an existing RecalcList, overwrite the RecalcList, or not create or update a RecalcList.

RecalcList Generation	
You can automatically create or update a RecalcList with files generated during automated Specify the RecalcList generation options for this SampleList below.	injections.
O not automatically create and update a RecalcList.	
C Create and update a new RecalcList.	
RecalcList name:	Browse
C Append to an existing RecalcList.	
RecalcList name:	Browse
Overwrite the Recalc List each time the SampleList Begins.	
OK Cancel	

If you select **Overwrite the RecalcList each time the SampleList Begins** the RecalcList is overwritten.

If you select **Append to an existing RelcalcList**, the new RecalcList has a number appended to the filename

QuickStart

QuickStart injects a single sample without using System Control directly.

You can customize QuickStart and set up instruments for routine use. Refer to online help for further details.

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



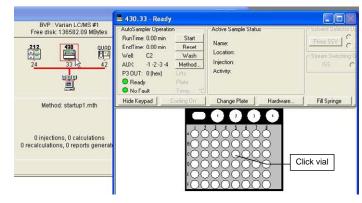
Enter information in the MS QuickStart window about your injection.

MS QuickStart - 1		
File Screen Options		
Instrument Num <u>b</u> er		1
Instrument Name	Instrument #	1
Operator Name	Operator	
<u>S</u> ample Name	Default Samp	le
Sample Description <u>1</u>		
Sample Description 2		
Primary Met <u>h</u> od		
C:\VarianWS\startup1.		
Folder for Data File Sto	rage	
C:\VarianWS		
Browse 430	L	
- Sample Type	Well/Vial	A1
C Baseline	# Injects	1
C Calibratio <u>n</u>	Wash Vol.	0
Analysis	Volum <u>e</u>	1
C Verification	<u>A</u> mount	1
Clear Coefficients	Fa <u>c</u> tor	1
	<u>M</u> ultiplier	1
AutoLink	<u>D</u> ivisor	1
	Level	1
	Inj. Mode Full Loop	-
		ardware
Start Stop	Help E	<u>x</u> it

AutoSampler Display

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

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



Running Priority Samples Using Inject Single Sample

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

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

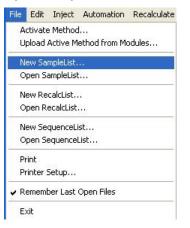
LC/MS or GC/MS Injecting Multiple Samples

Create SampleLists for different auto-samplers, and using more than one method for your injections.

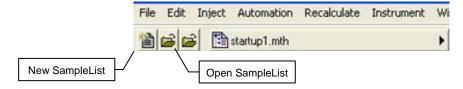
SampleLists in System Control

To inject multiple samples from System Control use a SampleList either from the File menu or from System Control.

To create a new SampleList: On the **File** menu, click **New SampleList** or click **Open SampleList** to select an existing one.



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



Generic SampleList

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

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

ieneric	SampleList: UNTITL	ED.SMP							.6
	Sample Name	Sample Type	Cal. Icycl	Inj.	Injection Notes	AutoLink	Amount Std (IS, N% only)	Unid I 🔺 Fac	Add
1		•							Insert
2	1	-							
3		-			1				Delete
4		-				2			Fill Down
5		-							Add Lines
[[1	+	Defaults

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

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

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

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

LC/MS - ProStar 410 SampleList

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

			Dilute, mix, a	an	d/or tran	sfer	\neg			
Dece	tar 410 SampleList: D	0,000								
1 19102	tar 410 sampterist: D	eno.smp						\backslash		
	Sample Name	AutoLink	Inj. Mode		lnj. Volume	Vial	Washes	Automix Routines	•	A <u>d</u> d
1	Default Sample	none	Partial Loopfill	•	10	1	1	none		Insert
2			No Injection Partial Loopfill							Inseit
3			Full Loop							Delete
4			ul Pickup							Fill Down
5				-						
6				-						Add Lines
7				-						Defa <u>u</u> lts
8				-					-	
•								•		
<u>B</u> egin	Suspend Resume							Data File	s	RecalcList

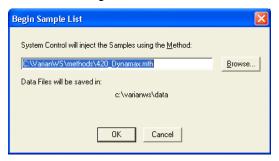
	Acti	ion	Amount	From		To		
1	Add	٣	10 ul	Reagent A	٠	Sample	Ŧ	
2	Mix	*	10 ul	1 tine	•		•	Add
3	Wait	Ŧ	0.50 min		-		•	-
4		-			•		*	loset
5		Ŧ			٠		* * * * *	Delete
6		-			•		•	Incert
7		Ŧ			٠		*	[mport.
8		•			•		*	
9		Ŧ			*		*	
10		-			•		•	
	Destina	lion 1	/iat none					
Au	tomix Fis	st Inje	ection Only					

Click Add Lines to add several lines to the SampleList.

Add Lines to ProSta	r 410 SampleList													X
Sample Name	Sample Type	Cal. level	lnj.	Injection Notes	AutoLink	lnj. Mode		lnj. Volume	Vial	Washes	Automix Routines	Prep Steps	Amount Std (IS, N% only)	Unid I Fac
Default Sample	Analysis 💌		1	none	none	Partial Loopfil	-	10	1	1	none		1	0
•														•
	of Lines to Add: 10 , Ne Names from: 1 nt Cancel		$\langle \rangle$, 	Number	√ials from: 1								
				Se	equent	tially num	۱b	er Sa	mple	Nam	es			

Press **Begin**, and you are prompted to select a Method. Use the active Method that was pre-selected, or click **Browse** to use another.

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



LC/MS - ProStar 420 and 430 SampleList

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

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

	Sample Name	Inj.	Injection Notes	AutoLink	Inj. Mode	lnj. Volume	Plat	Add
1	Default Sample	1	none	none	Partial Loopfill	10.0		Insert
2	Default Sample	1	none	none	Partial Loopfill	10.0		Inseit
3	Default Sample	1	none	none	Full Loop ul Pickup	10.0		Delete
4	Default Sample	1	none	none	User Program	10.0		Fill Down
5						•		
6							Not the	Add Lines.,

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

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

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

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

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

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

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

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

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

	Action		Positio	on	Amount	Speed	ġ.	Height	Comment	
1	Aspirate From	-	Sample	•	10.0 ul	3 (normal)	•	5 mm		Add
2	Dispense To	•	Sample	-	10.0 ul	3 (normal)	•	5 mm		
3	Aspirate From	•	Sample	-	20.0 ul	3 (normal)	•	5 mm		Insert
4	Dispense To	•	Sample	+	20.0 ul	3 (normal)	•	5 mm		Delete
5	Repeat	-		-	2 times		-	2 steps		
6	Wait	•		-	1.00 min		•			Import.
7	Rinse+Wash	+		-	100.0 ul		•			
8		•		-			•			
9		•		-			-			
10		•		-			•			
	Destination We Reagent A Via Reagent B Via	al: [1	None		- - -	Reage	nti	Plate: Samp C Vial: None D Vial: None	e Plate	
λ	tomix First Injec	tion	Oplu						ve As Default Autom	in Chan

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

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

When the User Program is selected as the Injection Mode, the following fields are disabled; Injection Volume, Wash Volume and Automix Routines. The User Program steps are used instead of the method parameters. You must use the User Program if the 10-ml syringe is selected. The following figure shows lists the User Program Actions. For each specified action, there could be several options such as Position, Amounts, Speed Setting, and Height.

	Action		Position	ı	Amount	Speed Setting		Height	Comment	
1 /	Aspirate From	•	Reagent A	•	10 ul	3 (normal)	•	5 mm		
2 [Dispense To	•	Sample	•	10 ul	3 (normal)	•	5 mm		
<u> </u>	Wait	•		•	1.00 min		•			_
4 F	Repeat	•		•	1 times		•	3 steps		
-	Wash	•		•	100 ul		•	ļ		-
-	/alve	•	Injector	•		Inject	•	ļ		
7 9	Syringe	•	Load	•	100 ul	3 (normal)	•	Į		
-	Compressor	•		•		Off	•			
_	Set Output	•	INJECT	•	,		•			
0		•		•			•			
0	Destination Via	al: n	one							
	Reagent A Via	al: C	:30	_		Reage	ent (C Vial: non	•	
1	Reagent B Via	il: n	one			Reage	nt D) Vial: non	e	
Start	Run on INJE	СТ	Marker							
Start	Run at End o	fU	ser Program						ave As Defa <u>u</u> lt Pro	gram Step
k	Cancel Us) 1	-	1	ve From Sa			Remove From S	

You can start the run, either on the INJECT Marker (step 9 in the above example), or at the End of User Program. Up to 240 steps can be programmed in one User Program. After adding all steps, enter a name for this User Program in the box next to Cancel (UserProg_1 in the above example), and press **OK**. The User Program is saved in the SampleList, and can be exported to other SampleLists. Or, use Import to bring User Programs from other SampleLists into the active SampleList.

ProStar 430 SampleList: UNTITLED.SMP Well / Vial Wash Volume User Program Amount Std Unid Pe (IS, N% only) Facto Automix Sample Name Plate Routine Add Default Sample 1 A1 300 0 none Insert Default Sample A1 300 0 2 none Default Sample A1 300 0 Delete 3 none Default Sample A1 300 0 4 none Fill Down A1 Default Sample 0 300 5 none 1 Add Lines.. 6 • f Defaults.. • Suspend Resume Data Files Recalcl ist Begin

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

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

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

GC/MS - CP-8400/8410 SampleList

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

	Sample Name	AutoLink	Vial	Injection Volume	Injectors Used	Amount Std (IS, N% only)	Add
1	Default Sample	none	0	1.0	Pos 1 🛛 👻	1	Insert
2					Pos 1		Insen
3					Pos 2 1 then 2		Delețe
4					2 then 1		Fill Down
5					Manual		
6					-		Add Lines
6			-		-	·	Defaults

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

	Sample Name	AutoLink	Vial	Injection Volume	Injecto Useo		Amount Std (IS, N% only)	Add
1	sample 1	none	0	1.0	Pos 2	•	1	Incent
2	sample 2	none	0	1.0	Pos 2	•	1	l <u>n</u> sert
3	sample 3	none	0	1.0	Manual	-	1	Delete
4	sample 4	none	0	1.0	Pos 2	-	1	Fill Down
5	sample 5	none	0	1.0	Pos 2	-	1	Fill Down
6	7		1			-		Add Lines

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

Injecto Used	I	2nd Injection	n	Injection Delay
1 then 2	•	Duplicate	•	0.5
	-	Duplicate		
	•	Advance Clean & Dup	,	
	•	Clean & Adv		

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

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

	Sample Name	2nd Sample Name	AutoLink	Vial	Injection Volume	2nd Inj Volume	Injectors Used	: 2nd Injection	Injection Delay	
1	Sample 1	Sample 2	none	5+6	1.0	2.0	1 then 2	Advance	▼ 2.0	
2								•	-	
3				1				•	-	
4				ĺ				-	-	
5				1				-	-	
6	7						•	-	-	
				1			-	-	-	•

Combi PAL SampleList

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

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

1 Standard 1 none none Automatic Tray1 2 Tray1 3 Tray1	
Tray2	- Insert
	Delete
4 ▼ Tray4	_ Fill Down
5 • •	-
6 • • •	Add Lines.

Default SampleList Entries

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

Sample Name Sample Type Cal. Inj. Injection AutoLink Inj. Mode Inj. Vial Wash Automix Routines								
Default Sample Analysis 🗸 1 none none Partial Loopfill 🗸 10 A1 300 none								
Save Cancel								

Note that neither volume nor rack and vial number is displayed, even if an AutoSampler is present.

Saving SampleLists for Later Use

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

Using More Than One Method for Injections

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

Changing the Method in the SampleList

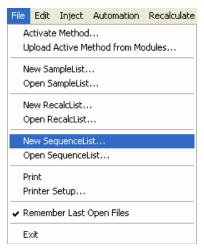
Change the Method by activating a Method in a SampleList row.

1 Default Sample Analysis 1 none none 1 none 1 none 1 none 1 none 1 <li1< li=""> 1 1<th></th><th>Activate Metho</th><th></th><th></th><th></th><th></th><th>[</th><th>Click Auto</th><th>oLink</th><th></th></li1<>		Activate Metho					[Click Auto	oLink	
2 Default Sample Analysis 1 none none Partial Lcopfill Default 3 Activate Method 420_dynamax Default Default 4 Verification Activate Method Default 5 Print Calib 6 New Calib Block		Sample Name	Sample	Туре	lnj.		AutoLink	Inj. Mode	<u> </u>	Add
2 Deroutin Sample Anaysis Image: Sample Particle Loopinit Particle Loopinit 3 Activities Method 420_dynamax Image: Sample Defo 4 Verification Image: Sample Image: Sample Image: Sample 5 Print Calib Image: Sample Image: Sample Image: Sample 6 New Calib Block Image: Sample Image: Sample Image: Sample 7 Audolinik Image: Sample Image: Sample Image: Sample	1	Default Sample	Analysis	-	1	none	none	Partial Loopfill	-	
4 Verification 5 Baseline Fill D 6 New Calib Block 7 Audolinik	2	Default Sample	Analysis	-	1	none	none	Partial Loopfill	-	Insen
5 Baseline 5 Print Calib 6 New Calib Block 7 Autolinik	3			hod 👻			420_dynama;		-	Delete
7 Autolink	5		Baseline Print Calib						-	Fill Down
Activate Method	7		Autolink						• •	Add Lines Defaylts

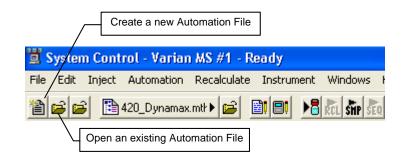
Enter M	ethod Name
Cancel	
	Enter M

Using the SequenceList Window

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



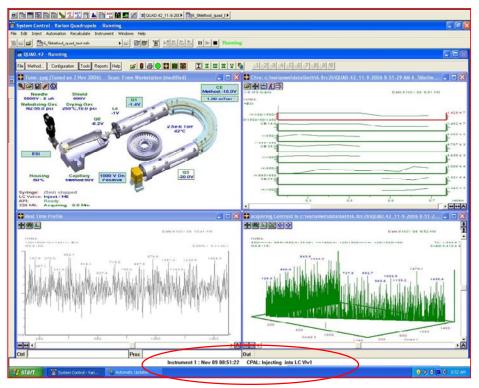
You can also create a new SequenceList or open one from the System Control toolbar.



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

				Enter the Metho	d and SampleList.
Select Action.	🗖 Sequ	enceList: test.seq	/		
		Action	Method /	Sample/RecalcList	· · · · · · · · · · · · · · · · · · ·
	1	Inject 👻	c:\varianws\420_dynamax.mth	c:\varianws\420_demo.smp	Add
	2	Inject 🚽]		l <u>n</u> sert
	3	Inject Recalc			Delete
	4	Print			
	6	Print Message Log Pump(s) Off			
	7	Lamp(s) Off			-
	•			•	Browse
	<u>B</u> egin	Suspend Resume			
			Browse for a Meth	nod or SampleList.	/

Monitor Run Status



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

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

Message Log

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

Message Log: MSGLOG1_7-26-2006_16_57_17.MLG	
Aug 30 14:00:37 Module CombiPAL.01: ATTACH Aug 30 14:00:37 Created Default Control Method for Module CombiPAL.01. Aug 30 14:00:48 Activating New SampleList UNTITLED.SMP	
Aug 30 14:00:323 Ins 1: Module 42: Module NOTREADY! Aug 30 14:10:23 Ins 1: Module 42: Module READY!	~

Message Log entries are stamped with the time and date.

Automated MS Report Generation

By adding Report sections to your Method, you can generate automated reports from System Control after each injection, after Recalculations, or by using Print

actions in the Sequence window. When Automated Printing is enabled, a checkmark appears in the front of the Enable Automated Printing menu listing. To disable automated Report printing during an automated sequence of injections or Recalculations, click **Enable Automated Printing** from the **Automation menu** to disable it and remove the check mark. SCII file generation is still performed, if selected in the Report Method section. When you disable automated printing, automation continues but no reports are printed.

Automation	Recalculate	Instrument W						
Begin Sam	npleList							
Begin Seq	uence							
Begin At S	Selected Samp	leList Line						
Begin At S	Selected Seque	ence Line						
Suspend A	Suspend Automation							
Resume Automation								
Stop Auto	Stop Automation							
Reset Mod	dules							
🗸 Enable Au	itomated Print	ing						

Stopping an Acquisition

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

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

Stop Automation - Stop the current run, resets all modules and suspends automation.

Resume Automation - Resume automation after suspension.

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

Automation	Recalculate	Instrument	W				
Begin Sam	pleList						
Begin Seq	uence						
Begin At 9	Selected Samp	leList Line					
Begin At 9	Selected Seque	ence Line					
Suspend Automation Resume Automation							
Stop Auto	Stop Automation						
Reset Mo	Reset Modules						
Enable Au	itomated Print	ing					

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

Operator: Sample Id: Default Sample	File name:	APR 11 2007 12	2-14
Sample Id: Default Sample		Browse	File naming methods
	Operator:		
	Sample Id:	Default Sample	
Notes:	Notes:		

Set a Collect Delay

LC/MS

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

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

GC/MS

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

Acquisition Method

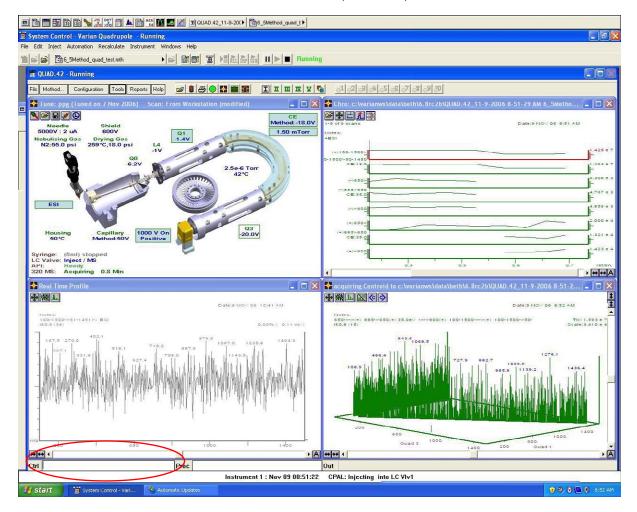
In **Method Builder**, open the **Acquisition Method.** Enable **Use delay** and enter the delay time in minutes.

Collect delay	
0.0	Min.

MS/MS Breakdown

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

The precursor ion can be viewed in the profile or centroid mode by entering **SW xxx** in the Ctrl text field (see below).



On the Tools menu, click MS/MS Breakdown.

122200	Reports	
Ste-21	t Macros	
Use	r pml	
Pml	Editor	
Plot	tic,readba	cks,
Ana	ilog output	of
MSN	15 Breakdo	wn
Bak	eout syster	n
Ove	ernight Star	ndby
Tro	ubleshootin	g
Inst	: setup/oth	ers

In GC/MS mode, your only choice is Q2 collision cell.

In LC/MS mode, you can select Q2 Collision Cell Breakdown, or API Capillary Breakdown.

Select optimizatio	on type	×
API Capillary	Q2 Collision cell	Cancel

The Create a breakdown curve window.

Create a breakdown c	urve	X
mass. It will generate and p	timize the collision energy for a given parent plot the relative intensity of the product ions v I time, use the 'opt_cid' PML)	s.
Parent mass	239	
🗐 Include pa	arent -> parent in breakdown curves	
C Auto find p	product masses from mass 50 to 230	,
Use these	product masses	
Mass 1	197.0	
Mass 2	195.0	
Mass 3	175.0	
Mass 4	132.0	
Mass 5	130.0	
Collection speed C Fast Normal	Graph scale Smooth curves	
Add ions to scan method Save Append	Image: Text constraints Browse mest ions to method M6G_gluc_recalc	•
Method folder:C:\Varian\	WS\Examples\1200 MS Data Files\	
Turn off syringe pump al	fter collecting breakdown curves	
Start Redraw S	itop Turn on CID gas Apply Ca	ncel

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

The breakdown curves are displayed.

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

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

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

If you select API capillary, do the following after the **Create a breakdown curve by scanning the API capillary** window opens.

	to optimize the API capillary of the product ions vs. capil 	lary volt	age.	
C Auto find pro	duct masses from mass 1	0.0	to 4	400.0
Ose these mage	asses			
Mass 1				
Mass 2				
Mass 3				
Mass 4				
Mass 5				
Collection speed	Graph scale	0.000	mooth c	
C Fast	Absolute		Smoo	
Normal	C Scale each trace	, E		Points
Add ions to scan meth	A CONTRACTOR OF A CONTRACTOR OFTA CONTRACTOR O	trowse	 recalc	
• Append	rianWS\Examples\1200 MS			
	mp after collecting breakdo			

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

The breakdown curves are displayed.

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

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

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

Analog Channels

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

Select Analog output of from the Tools Menu

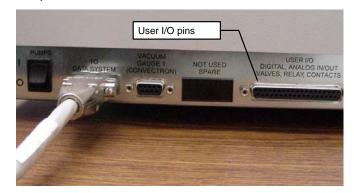


The Analog Out widow opens.

Analog Out (Once per scan)
Analog output #1 (User I/O connector-> Signal = pin 14 , Gnd = pin 32 +/-5 Volts)
TIC (Total Ion current) Gain for TIC or mass trace 0.001 C Area of mass 0.0
C Any PML expression (should return a value between -5 and 5)
Example: readback(55) * 1000
Analog output #2 (User I/O connector-> Signal = pin 33 , Gnd = pin 15 +/-5 Volts)
FIC (Total Ion current) Gain for TIC or mass trace 0.001
C Area of mass 0.0
C Any PML expression (should return a value between -5 and 5)
Example: area(219)
Apply OK Cancel

To create an Analog signal output:

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



Automation File Editor

Overview

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

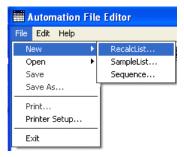
NOTE: SampleLists and Sequences that are active and running in System Control cannot be accessed in the off-line Automation File Editor.

Accessing the Automation File Editor

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

Create or Edit a RecalcList

Either select a New RecalcList or Open an existing RecalcList from the File menu.



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

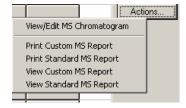
-	📰 🛐 🟗 💊 🗊 🏰 🔏 🔳 4000.56031.SMS 🕨 🖺 Cottest_Extr									
	mation File Editor - [Pesticide.rcl]									
Edit	t Help									
) 🖻										
Pesti	icide.rcl - RecalcList									-
	Data File	Sample Name	Sample Type		Cal. level	lnj.	Recalc Notes	AutoLink	Amou (IS, N	Add
1			New Calib Block	•						Insert
2	c:\varianws\data\version_631\pesticide_linearity\flow_5ml\pest_2ng_5ml_1.sm	Pest_2ng_5ml	Calibration	-	2 1	1	none	none		
3	c:\varianws\data\version_631\pesticide_linearity\flow_5ml\pest_1ng_5ml_1.sm	Pest_1ng_5ml	Calibration	•	3 1	1	none	none		Delete
4	c:\varianws\data\version_631\pesticide_linearity\flow_5ml\pest_500pg_5ml_1.	Pest_500pg_5ml	Calibration	-	4 1	1	none	none		Fill Dov
5	c:\varianws\data\version_631\pesticide_linearity\flow_5ml\pest_200pg_5ml_1.	Pest_200pg_5ml	Calibration	•	51	1	none	none		
6	c:\varianws\data\version_631\pesticide_linearity\flow_5ml\pest_100pg_5ml_1.	Pest_100pg_5ml	Calibration	•	61	1	none	none		Default
7	c:\varianws\data\version_631\pesticide_linearity\flow_5ml\pest_50pg_5ml_1.s		Calibration	•	71	1	none	none		Browse
	c:\varianws\data\version_631\pesticide_linearity\flow_5ml\pest_20pg_5ml_1.s		Calibration	-	81		none	none		Papart
8	c:\varianws\data\version_631\pesticide_linearity\flow_5ml\pest_10pg_5ml_1.s	Pest 10ng 5ml	Calibration	-	91	1	none	none		Report
	c. Waital We sublid Top Typestic de_inteality now_onit typest_ topg_onit_1.	rest_repg_onn								

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

AutoLink - Enter post calculation operations.

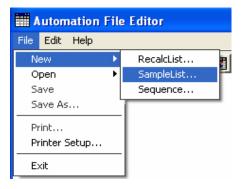
Report - Generate a report for the selected data file. Note that if a data file is not highlighted in the Data File column, no report is generated.

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



Create or Edit a SampleList

Either select a New SampleList or Open an existing SampleList from the File menu.



Select a folder for the SampleList, enter a name, and click Save.

Create a new Sam	ıpleList File		? 🗙
Save in: 🛅 Varian	WS	1	💣 🎟 -
500-MS Methods 1200Service 1200sys 4000Service 4000Sys Autotune Logs	ChromExamples data Examples Library Manuals methods	MSGLOG MSTutorials SatSys Service SYSLOG System	UserPML WSDataFiles kodiak.smp test.SMP
<			>
File name: Untitle	ed.smp		Save
Save as type: Samp	oleLists (*.smp)	•	Cancel
			Recent Files >

Select the autosampler and click **OK**.

Sele	ct SampleList Section Type		×
	Please select a SampleList Section Type		
	8200 StandAlone AutoSampler 8400 AS on 3900	^	
	8400 AutoSampler 8410 AS on 3900		
	8410 AutoSampler CombiPAL AutoSampler Generic	~	
	OK Cancel]	

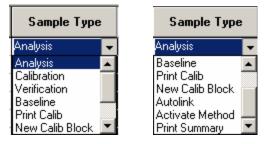
Size the Spreadsheet columns by dragging their borders with the left mouse button. Right-clicking a column header displays formatting options. The Sample Name column does not scroll.

	Sample Name	Sample Type	Cal. level	Inj.	Injection Notes	AutoLink	Vial	Injection Volume	Injectors Used	Amount Std (IS, N% only)	Unid Peak Factor	Multiplier	A <u>d</u> d
1									-				Insert
2									-				
3									-				Delete
4 5		-											Fill D <u>o</u> wn
5		÷											Add <u>L</u> ines.
7		-							+				Defa <u>u</u> lts
B		-							-				
9		-							•				Hardware
0		•			1				-				

SampleList Fields

Sample Name - Enter the sample name. Create sample names by clicking **Data Files**. If only '%s' is listed in the Data Files the sample name is as you entered it.

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



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

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

Injection Notes - Enter notes about the sample.

	×
<u>R</u> evert	Cancel
	<u>R</u> evert

AutoLink - Refer to the 'Specifying Data Handling Parameters' section in this manual.

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

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

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

Inject the Sample using the Method:	
C:\VarianWS\Coltest_External.mth	Browse

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

Other Fields

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

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

Delete - Deletes the currently active line.

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

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

Add Lines to 8400 SampleList													
Sample Name	Sample Type	Cal. level	lnj.	Injection Notes	AutoLink	Vial	Injection Volume	Injectors Used	Amount Std (IS, N% only)	Unid Peak Factor	Multiplier	Divisor	MultiChannel MultiStandard
Default Name	Analysis 🔹 👻		1	none	none	0	1.0	Pos 1 💌	1	0	1	1	none
Default Name Analysis I													

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

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

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

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

Specifying the Data File Name and Path

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

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

Data File Generation	×
	d by detector modules using this SampleList. the file already exists. Do not include the file
Directory for Data Files	Data File names
C:\ C→ VarianWS	%d-%s-%i
🗁 4000Module	Example:
	6-28-2004-Sample 1-1
V	Use the following symbols to enter the corresponding variable data to the file
New Folder	name.
	%s = Sample ID
	%i = Injection number %d = Date
Drives:	%m = Detector Module name
	%t = Injection Time
OK	Cancel

Select the data file directory from the left side. Create a file name specification on the right. You can combine text entry with the "%" variable symbols to specify file

names that contain sample injection specific information. An example of the file name is updated as you enter the file name specification.

Specifying a RecalcList

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

RecalcList Generation										
You can automatically create or update a RecalcList with files generated during automated injections. Specify the RecalcList generation options for this SampleList below.										
C Do not automatically create and update a RecalcList.										
Create and update a new RecalcList.										
RecalcList name: c:\varianws\untitled.rcl Browse										
C Append to an existing RecalcList.										
RecalcList name: Browse										
Overwrite the Recalc List each time the SampleList Begins.										
OK Cancel										

Changing Default SampleList Entries

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

To change the default values:

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

Set 8400 SampleList [iet 8400 SampleList Defaults													
Sample Name	Sample Type	Cal. level	lnj.	Injection Notes	AutoLink	Vial	Injection Volume	Injectors Used	Amount Std (IS, N% only)		Multiplier	Divisor	MultiChannel MultiStandard	
Default Name	Analysis 💌 🔻		1	none	none	0	1.0	Pos 1 💌	1	0	1	1	none	
<u>S</u> ave Cano	el													

Using More Than One Method for Injections

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

Changing the Method in the SampleList

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

	Sample Name	Sample Typ	e	Cal. level	Inj.	Injection Notes	AutoLink	Vial	Injection Volume	Injectors Used	Add
1	Sample_1	Analysis	-		1	none	none	0	1.0	Pos 1 💌	Insert
2	Sample_2	Analysis	•		1	none	none	0	1.0	Pos 1 💌	
3	Sample 3	Analysis	-	Į.	1	none	none	0	1.0	Pos 1 💌	Delețe
4	_	Activate Method	_	Į.			none			•	Fill Dowr
5	Sample_4	Verification Baseline	•		1	none	none	0	1.0	Pos 1 💌	
6		Print Calib								<u> </u>	Add Lines
7		New Calib Block	:							<u> </u>	Defaults.
8		Autolink Activate Method	-							<u> </u>	Hardware
9			-							<u> </u>	Hardware
0			-							<u> </u>	

Select Activate Method from the Sample Type cell.

Click **AutoLink** in the row that you are working. The Activate Method widow opens.

Activate Method	
Method PathName	
C:\VarianWS\NewMethod.mth	
Browse	OK Cancel

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

	Sample Name	Sample Type	•	Cal. level	lnj.	Injection Notes	AutoLink	Vial	Injection Volume	Injectors Used	Add
1	Sample_1	Analysis	-		1	none	none	0	1.0	Pos 1 💌	Insert
2	Sample_2	Analysis	그		1	none	none	0	1.0	Pos 1 💌	
3	Sample 3	Analysis	-		1	none	none	0	1.0	Pos 1 👱	Deleţe
4		Activate Method	-				NewMethod.n			-	Fill D <u>o</u> wn
5	Sample_4	Analysis	그		1	none	none	0	1.0	Pos 1 👻	Add Lines
6	-		•							<u> </u>	Add Lines
7	-		- -							<u> </u>	Defa <u>u</u> lts
8 9	-	_	-							÷	Hardware.
10	-	-	÷							<u> </u>	

Specify any number of Methods in the SampleList.

Create or Edit a Sequence

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



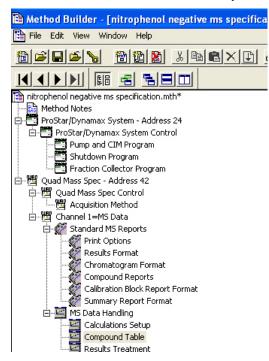
The Sequence window opens.

	Action		Method	Sample/Recale	
1	Inject	-	c:\saturnws\gcexamples\another.mth	c:\saturnws\gcexamples'	Add
2		•			l <u>n</u> sert
3		-			Delete
4		-			
5		-			
6		-			
7		-			
8		-			Browse
9		-			
10		-			

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

Compound Table

In the Method Builder tree, click **Compound Table** under MS Data Handling.



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

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

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

Creating a Compound Table

- 1. Click Build Compound List.
- 2. Click each peak to create an entry.
- In the Method Editor, click Import Compound List, and click Select to put your compound list into the method.

Note: You can double-click a cell to display more information.

16 13		Quan Ion	Calculations	Integration	Identification	
3	2,4-Dimethylphenol	107.0, C:1	Linear, Ignor, 1	0.25, W:4.0, S:20	0.20, Spec	107.0, 122.0, 121.0
	bis(2-Chloroethyl)ether	93.0, C:1	Linear, Ignor, 1	0.25, W:4.0, S:20	0.20, Spec	93.0, 63.0, 95.0
68	Heptanediamide, N,N'-d	105.0, C:1	Linear, Ignor, 1	0.25, W:4.0, S:20	0.20, Spec	105.0, 77.0, 122.0
19	2,4-Dichlorophenol	162.0, C:1	Linear, Ignor, 1	0.25, W:4.0, S:20	0.20, Spec	162.0, 63.0, 98.0
78	1,2,4-Trichlorobenzene	180.0, C:1	Linear, Ignor, 1	0.25, W:4.0, S:20	0.20, Spec	180.0, 182.0, 109.0
73	Naphthalene-D8	136.0, C:1	Linear, Ignor, 1	0.25, W:4.0, S:20	0.20, Spec	136.0, 108.0, 52.0
26	Naphthalene	128.0, C:1	Linear, Ignor, 1	0.25, W:4.0, S:20	0.20, Spec	128.0, 102.0, 127.0
'8	4-Chloroaniline	127.0, C:1	Linear, Ignor, 1	0.25, W:4.0, S:20	0.20, Spec	127.0, 129.0, 92.0
21	Hexachlorobutadiene	225.0, C:1	Linear, Ignor, 1	0.25, W:4.0, S:20	0.20, Spec	225.0, 227.0, 223.0
7	73 26 78 21 21 21 21 22 22 22 22 22 22 22 22 22	Naphthalene-D8 Naphthalene Naphthalene 4-Chloroaniline	Naphthalene-D8 136.0, C:1 26 Naphthalene 128.0, C:1 78 4-Chloroaniline 127.0, C:1	Y3 Naphthalene-D8 136.0. C:1 Linear. Ignor. 1 26 Naphthalene 128.0. C:1 Linear. Ignor. 1 78 4-Chloroaniline 127.0. C:1 Linear. Ignor. 1	Naphthalene-D8 136.0, C:1 Linear, Ignor, 1 0.25, W:4.0, S:20 Naphthalene 128.0, C:1 Linear, Ignor, 1 0.25, W:4.0, S:20 78 4-Chloroaniline 127.0, C:1 Linear, Ignor, 1 0.25, W:4.0, S:20	Naphthalene-D8 136.0, C:1 Linear. Ignor. 1 0.25, W:4.0, S:20 0.20, Spec R6 Naphthalene 128.0, C:1 Linear, Ignor, 1 0.25, W:4.0, S:20 0.20, Spec R8 4-Chloroaniline 127.0, C:1 Linear, Ignor, 1 0.25, W:4.0, S:20 0.20, Spec

Compound Attributes

The following shows the **Compound Attributes** tab view after the retention time 7.613 was double-clicked. The Chromatogram and Spectrum Displays are on top and the bottom part has fields. After you select **Quan lons**, other than the RIC, (for example, in the Build Compound Table dialog in MS Data Review or in the Quan lons Tab view) use the selected Quan lons for Plot parameters.

Add information, such as Compound Name and CAS Number, during the peak addition process.

Compound Attributes	Quan Ions Calc	ulations Integration	Identification	Ref. Spectrum
7.316 2,4-Dimethylphenol	107.0, C:1 Linear,	Ignor, 1 0.25, W:4.0, S:2	0.20, Spec	107.0, 122.0, 12
400- 300- 200- 100- 7.25 7.75 1 Scans 537 574	SMS 107.0 (Chan: 1) 8.00 8.25 8.50 8.75 minutes 6.7 22-8.91, El Auto 6.11 6.48	100%	77.0 150 61725 316 min. Scan: 54 77.0 9 394	7.0 019 12 lon: 220 us 7.0 99
Compound Attributes		Compound Type		
Retenti <u>o</u> n Time (min):	7.316	C Internal Standard	🔽 Acti <u>v</u> e	
Compound Name:		Analyte	RR <u>I</u> Reference	
2,4-Dimethylphenol			Identification Re	eference Pk
CAS Num <u>b</u> er:	105-67-9	IS to <u>U</u> se:		_
		<u>G</u> roup Name:		_
		Previous <u>N</u> ex	tt <u>C</u> lose	<u>R</u> estore

Edit Name, CAS Number, Retention Time

You can edit the Compound Name and CAS fields.

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

Identify Internal Standards

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

Identify Group Members

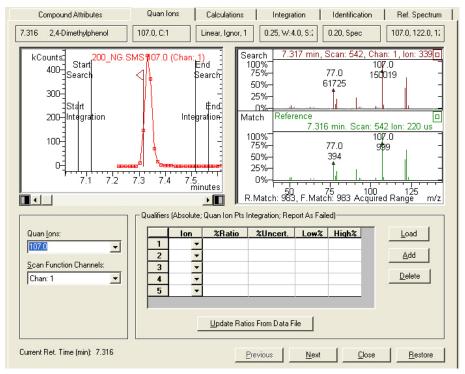
Sometimes target compounds are identified as a member of a group of compounds (for example, Trihalomethanes (THM), alkyl aromatics, etc.).

Enter the desired name in the Group Names field.

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

Quan lons

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



Edit Quan lons

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

]
1

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

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

Select lons to Plot				X
Edit Ion Formula The valid ion range is from 2.0 to IONS: RIC	2000.0.		STATUS: V	alid Ion Formula
Show Format and Examples		Help	OK	Cancel
Format and Examples				
Specify an ion selection by combini				
of the following items, with the '+' a	nd ¹⁴ operators.			
 Individual Ions (e.g., 40.0) 				
- Range of ions (e.g., 40.0:60.0)				
- All ions: RIC				
Examples: 28.0	(Plot ion 28.0 only.)			
40.0:450.0	(Plot ions 40.0 through 450.0.)			
RIC-128.0	(Plot all ions except ion 128.0.)			
91.0+128.0	(Plot ions 91.0 and 128.0.)			
60.0:450.0-128.0	(Plot ions 60.0 through 450.0 except ion 128.0.)			

Edit Retention Time

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

Look at Other Compounds

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

Select Qualifier lons

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

	lon		%Ratio	%Uncert.	Low%	High%	Load
1	63.0	-	87.5	20.0	67.5	107.5	1
2	93.0	-	73.0	20.0	53.0	93.0	Add
3	122.0	-	62.0	20.0	42.0	82.0	-
4		-					<u>D</u> elete
5		-					

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

The Qualifiers Table has the following fields:

lon - Click in the Ion field to see the choices.

Ratio - Shows the intensity of the qualifier ion as a percentage of the chosen Quan ion(s).

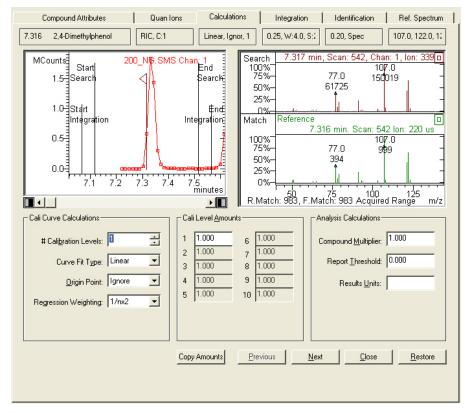
%Uncert. - Allowed percentage deviation from the Ratio. You can change the default of 20%. The % Uncertainty allowable range dependents on the Ion Ratio Type setting in the Calculations Setup Dialog (Absolute % or Relative %).

Low% and High% - For ion 63, the top line in the previous example, and the allowed range for the ratio is $87.5.0 \pm 20\%$ (absolute). Therefore 67.5% is the Low% value and 107.5% is the High% value area.

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

Calculations Tab

Click the Calculations tab to display the following.



Enter Number of Calibration Levels and Amounts

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

Cali Curve Calculations	Cali Level Amounts	Analysis Calculations
# Cali <u>b</u> ration Levels: 6 🛨	1 10.000 6 160.000	Compound <u>Multiplier</u> : 1.000
Curve Fit Type: Linear 💌	2 20.000 7 1.000 3 40.000 8 1.000	Report <u>Threshold</u> : 0.000
<u>O</u> rigin Point: Ignore	4 80.000 9 1.000	Results <u>U</u> nits: ng/mL
Regression Weighting: 1/nx2	5 120.000 10 1.000	

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

Quan Ion	Calculations	Integration
95.0, C:M	Linear, Ignor, 1	0.25, W:4.0, S:20
61.9, C:M	Linear, Ignor, 1	0.25, W:4.0, S:20
78.0, C:M	Linear, Ignor, 1	0.25, W:4.0, S:20
82.9, C:M	Linear, Ignor, 1	0.25, W:4.0, S:20

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

Select Curve Fit

Select the desired curve fit from the list.

Cali Curve Calculations—		
# Cali <u>b</u> ration Levels:	1	÷
Curve Fit Type:	Linear	•
<u>O</u> rigin Point:	Linear Quadratic Cubic	

For most calibration curves, use either Linear or Quadratic.

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

Security Administration

Overview

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

- Passwords
- Application Locking
- File Revision Settings

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



Passwords

	ation
asswords	Application Locking File Revision Settings
Passwor	d for this application
You may this appli	set, change or remove the password required to ente cation.
	Change Password
Change I	Method Passwords
Methods.	set or change passwords required to save changes to Click on the button below to select the Method, and
then moc	lify the password.
Remove You may	Select Method Method Passwords remove passwords required to save changes to Click on the button below to select the Method.
Remove You may	Select Method Method Passwords remove passwords required to save changes to

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

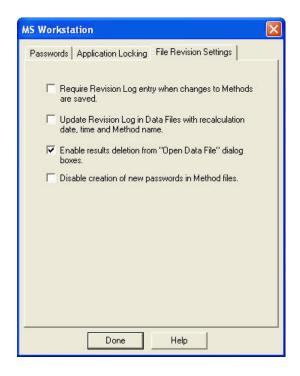
Application Locking

MS Workst	ation		×
Passwords	Application Locking	File Revision Settings	
Select button. MS Dai MS Dai MS Dai MS Dai Star To Star To System	ed Applications applications you wish t ta Review - [Plot Chron ta Review - Plot Chrom ta Review - Plot Chrom n Manager olbar Control - MS - Not Rea	to lock and click on the Lock natogram atograms Lock	
1.		unlock and click on the	
	Done	Help	

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

File Revision Settings

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



Configuring HPLC Modules

Overview

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

Refer to Data Acquisition with LC Control, part number 391473200 and 212-LC Operation Manual, part number, 395410300 for details.

Configuring GC Modules

Overview

Since the 3800 GC communicates with the Workstation over a standard Ethernet connection, your system can easily be expanded from a single 3800 GC/single Workstation configuration, to multiple 3800 GC/Workstations, to a fully networked lab with a virtually unlimited number of GCs and Workstations. The term "Ethernet" refers to the cables and interface cards that connect devices to the network. If you are connecting your 3800 GC to an existing Ethernet network, you need to know which type of cable to use. Refer to the *Communications* section of the 3800 GC Operator's Manual.

The 3800 GC uses TCP/IP (Transmission Control Protocol / Internet Protocol) to communicate over the Ethernet network. Since the 3800 GC uses TCP/IP to communicate with the Varian MS Workstation, the Workstation PC and the 3800 GC need unique IP addresses—the addresses that are used to identify each networked TCP/IP device.

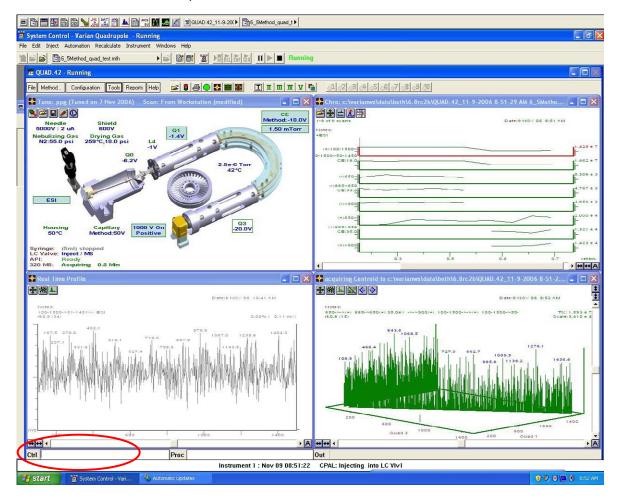
Refer to Data Acquisition with 3800 GC Control, part number 391473100, for detailed information about how to acquire data, build methods, and operate the 3800 GC with your Varian MS Workstation. This manual also describes the configuration of the 3800 GCs for standard Ethernet communication with System Control.

PML

Overview of PML

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

Simple Commands



Simple commands can be entered in the CTRL field.

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

CANCEL stops the Paw macro running at the top level.

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

PML Syntax

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

The names can contain letters, numbers, or underlines, but they must begin with a letter.

Run a macro by typing the name of the command lines of the instrument window (CTRL) or including the name in another macro. You can send arguments to a macro and it will return a value.

Paw Macros Consist of Statements:	Examples:
Action or function keywords:	OFF DOZE(2.5)
Macro calls:	CGON SW(219)
Assignment statements:	DETECTOR = 1000 DETECTOR += 50 DETECTOR -= 50 x = COS(PI)
Conditional Statements:	IF (WIDTH > 10) ELSE WHILE (x < 100 & y <= 100) UNTIL (x = 100 y != 100) REPEAT 100 REPEAT
Completing Statements:	END terminates a conditional statement
	RETURN(n) returns from a subroutine with result n
	CANCEL stops the paw macro running "at the top level"
	QUIT stops all paw macros
Printing statements:	?DETECTOR prints the current detector value on the display.
	"Hello" prints Hello on the display.

The Statements Refer To:

e.g.	20, -3.5, 1000H
e.g.	DETECTOR
e.g.	COS
e.g.	FISH
e.g.	STANDBY
e.g.	X,Y
e.g.	%1,%2,%3,%4,%5
	e.g. e.g. e.g. e.g. e.g.

Notes

- 1. Statements are separated from each other by colons, semicolons, or line breaks.
- 2. Conditional statements must have a matching END statement, e. g.:
 - if (x < y) & ~(x = 2) : fish : else : scanlens : end
 - if x = 3 : sw(502) : end
 - i = 1 : repeat 100 : sn = i: list(i) = tic : i + = 1 : end

However, END statements at the bottom of a PAW Macro can be deleted.

- 3. Printing statements (using ? and "") can be strung together. They are terminated with the keyword CR (carriage return).
- 4. Some keywords create text like the printing statements using ? and "."

GET_FILENAME LIB_FORMULA LIB_NAME LIST_TO_STRING SAMPLE_NAME STRING_RESTORE SUB_FILE_NAME VERSION

5. Some keywords re-route the text created by printing statements (using ? and ") to other places than the display.

DACS_RESTORE	: "file name" : CR
DACS_SAVE	: "file name" : CR
FILE_APPEND	: "file name" : CR
FILENAME	: "file name" : CR
FILE_OPEN	: "file name" : CR
IONS_RESTORE	: "file name" : CR
IONS_SAVE	: "file name" : CR

LCD	: "message" : CR
LIB_FIND	: "compound name" : CR
LIST_RESTORE	: "file name" : CR
LIST_SAVE	: "file name" : CR
MSGBOX	: "label text" : CR : "default": CR:
"Macro": CR	
PICT_LABEL	: "label text" : CR
PICT_TITLE	: "title text" : CR
STRING_SAVE	: "text" : CR (ten user strings)
STRING_TO_LIST	: "text" : CR
SUB_NAME	: "text" : CR

- 6. Statements may include comments. A # ends the statement and starts the comment, e.g., :DETECTOR += 10 # raise the detector to make the peak bigger.
- All numerical values referred to in PAW Macros are real numbers. Usual algebraic syntax is allowed:, e.g., x = (sin(y) + cos(sqrt(detector))) / (30 * month + day).
- 8. When parameters are passed to macros, they are referred to within the macro as %1, %2, %3, %4 and %5. e.g., if the macro TIMES is defined as ?%1 : "times" : ?%2 : "equals" : ?(%1 * %2) : CR and you type "TIMES 7 9" and the instrument will print out "7 times 9 equals 63". NOTE: %1 %5 can be used as local variables within any macro.
- 9. When passing parameters to a macro or keyword, you can leave out parentheses at the top level.

All these are valid statements:

FISH(3) FISH 3 FISH 3 2 FISH 3,2 FISH(3,2) When assigning a value to a variable or parameter you can leave out the = sign. DETECTOR = 1000

DETECTOR 1000

but: "lens(1) = 100" is ok while "lens 1 100" is ambiguous.

10. When using printing statements on the control line, or if the string you type starts with? or " or VERSION, you don't have to type the terminating CR.

System Paw Macros

- 1. When the Status Window is opened, a Ctrl: PML (default: INIT) and a Proc: PML (default: QUAN_INIT) are both run.
- 2. In the Collect menu (toolbar start button) a Ctrl: PML is defined which runs when the file being collected is opened.
- 3. In the queue menu (Collect Queue edit button) a Proc: PML is defined which runs when the file being collected is closed.
- 4. A Windows application outside the instrument can request a PML through the windows DDE mechanism.
- 5. Using the MSGBOX keyword you create and run PMLs.
- 6. Some PMLs run when you click on buttons or menu items:

File menu Reset: INIT

File menu Standby: STANDBY

Status control menu: CGON CGOFF CION CIOFF CIDON CIDOFF

AutoTune menu: ATUNE1 ATUNE2 ATUNE3 ATUNE4 ATUNE5 ATUNE6

Diagnostic menu: DIAGNOSTIC(test_number)

Tune Table menu optimize button: OPTIMIZE

Status probe button: PROBE_MAIN

Species Boiling Pt. Range menu compute button: SHELL

Clicking in Chro: CHRO_CLICK(sn,rt,type_rt + (10*type_sn) + (1000*make_substance))

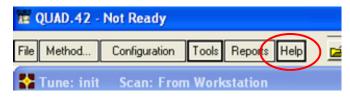
(click on the CHRO scales button to see where type_rt,type_sn, and make_substance are defined)

Other popular PMLs are:

BL	PAR
DAU	QIMS
FM	Q3MS
LM	SCAN
MIXED	SW
NL	

Help Files for PML

Click **Help** in the System Control window to open the Paw Guide.





The Quad MS window is your window to the instrument. It contains several views, each providing a different way to view or interact with the instrument. It also contains a toolbar, and two command lines on which you may type Paw Macros to control the instrument or process data.

Toolbar Buttons			
File	Method	Configuration	Tools
Reports		12	
Help	🖻 View File	Collect File	Print .
Instrument On / Off	-	•	
Instrument	🖬 Scan Editor	<u> Auto Tune</u>	I II II II II V View setups
🖬 Select Views			
Views			
A_ Prof	LLL Cent	DInstrument	Readbacks
LLL Spec			
	Map	الليليا بالاليال Library	Ι23 Σσ <u>List</u>
Pict			
Paw Macro Keywol	rds		

<u>Paw Macro Keywords</u> <u>Diagnostic Paw Macro Keywords</u> <u>Paw Macro Syntax</u> <u>System Paw Macros</u>

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Some PML Procedures

The Cioff.pml macro closes the CI gas valve, prints "Evacuating CI Gas (takes 5 seconds)" in the status area of the taskbar, opens and closes the vent valve, and prints "CI gas off" in the status area of the taskbar.

CIOFF.pml

valve 2 = 0	# close CI valve
"Evacuating CI Gas (takes 5 seconds)";cr	#printing statement, terminated with the keyword CR (carriage return)
doze 1	#wait one second
valve 4 = 1	# open CI vent valve for 0.2 seconds
doze .2	
valve $4 = 0$	# close vent valve for one second
doze 1	
valve 4 = 1	# open vent for 3 seconds
doze 3	
valve $4 = 0$	# finally close vent
"CI Gas off!";cr	#printing statement, terminated with the keyword CR (carriage return)

The LEAK.pml assists in finding vacuum system leaks. It sets a series of masses from a compound or mixture used for leak detection. First. the Pict view window is cleared, the title in the Pict window is set, centroid mode is set, mass range is set, the parameters are optimized to prevent saturation, and a series of mass intensities are plotted while the user sprays a gas at possible leak locations.

LEAK.pml

pict_clear	# clear the picture/graph window
pict_title:"1->mass 18, 2->mass 28, 3->mass 33, 4->mass 45, 5- >tic":cr	#Sets the title in the pict view
cent	#Go to centroid mode
fm 10	#Set first mass (FM) to 10
lm 50	#Set last mass (LM) to 50
optdet	#Optdet runs opt_detector.pml to prevent detector saturation after each scan.
repeat	#repeat items below
fish	#go get one scan of data
pict(,area(18),1)	#get area of mass 18 and plot point in pict view position 1
pict(,area(28),2)	#get area of mass 28 and plot point in pict view position 2
pict(,area(33),3)	#get area of mass 33 and plot point in pict view position 3
pict(,area(45),4)	#get area of mass 45 and plot point in pict view position 4
pict(,tic,5)	#get area of mass total ion current (tic) and plot point in pict view position 5
end	

Mixed.pml gets one scan in centroid data and one scan of profile data.

MIXED.pml. When Prof and Cent views are selected in the window, both real time centroid and Profile data is observed.

Repeat	#repeat items below
Prof	#set to scan of profile data
Fish	#go get one scan of data
Cent	#set to scan of centroid data
Fish	#go get one scan of data
End	

PML Editor

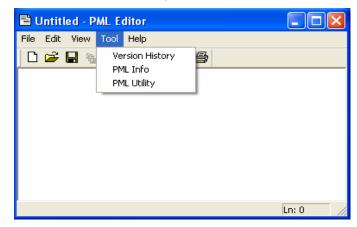
The **PML Editor** is used for creating and editing PMLs for the 300 Series software. The PML Editor allows access to the factory PML files; however, if a factory PML is modified it will then be saved as a user PML in the UserPML directory.

Accessing the PML Editor

File Method ... Configuration Tools Reports Help Quit Macros 🚰 Tune: init 🛛 Scan: Fron User pml... **2** Pml Editor... Trans. Line Plot tic, readbacks, ... 00 Analog output of... MSMS Breakdown... Bakeout system Overnight Standby Troubleshooting... Cal 100 P Inst setup/others...

Click **Tools** in the Quad module window to display the PML editor.

The PML editor window opens.



- Varian PMLs are stored in c:\varianws\1200sys\PML directory.
- User created PMLs or modified factory PMLs are stored in c:\varianws\UserPML directory.

• The Status Bar of the PML Editor displays the line number of the current cursor position.

📑 abort.pml MSWS 6.42 - PML E	Editor
<u>File E</u> dit <u>V</u> iew Tool <u>H</u> elp	
🗋 🗅 📂 🔚 🍇 👗 🛍 🛍 🗠	4
abort_request = 1.0 # The C Code will then invok	ppropriate state and then call QUIT 1 s
if (bl_running) bl_running baseline average avmode scan_time	Selected line number = 0 = bl_baseline = bl_average = bl_avmode = bl_scan_time
Ready	Ln: 7 /

• The Tool menu has three menu items:

Version History: If the 21CFR11 application is enabled, click this to display the version history of the currently open PML.

Version History	
Version History:	
C:\VarianWS\UserPML\log_all.PML, Versions 1 to 2	
Version 1 saved on 3/18/2005 9:53:42 (GMT-8:00) by Yu-Hsing Chiu	
PML version control creation	
Version 2 (Tip) saved on 3/18/2005 9:54:37 (GMT-8:00) by Yu-Hsing Chiu	J
add one more comments	
OK	

PML Info: Display the PML path name, release version number, and any descriptions that have been in the PML header section. (Lines begin with ##).



PML Utility: Use this to perform syntax checking of the currently open PML and produce a call tree, PML keywords and User Variables defined in the PMLs. For the keywords listed, user can select and use F1 to get online help about the keywords.

In the right part of the utility dialog box, user can enter a specified keyword, and find out the PMLs contain this keyword.

🛿 Show user variables 🔽 Show keywords 🗖 Show 'all-in-one'	Show direct references only
ABORT ABORT ABORT ARSTORE_PRE_AUTOTUNE_STATE MAKE_TUNE_NAME MAKE_DATE_STRING MAKE_TIME_STRING ASTANDBY_EXIT AIS API CDON CDOFF CDOFF COFF GOFF GOFF BL_AVERAGE BL_AVERAGE BL_SCAN_TIME BL_CENT SL_CENT SL_CENT SL_SCAN_TIME SL_SCAN_TIME	The Macro abort is used directly by pmls: autotume opt_coarse_slope opt_detector_gain opt_edr plot_breakdown plot_breakdown_cap
uccesses	
Compiled abort Compiled alloff Compiled alloff Compiled api_lid	
roblems	