Varian, Inc.
2700 Mitchell Drive
Walnut Creek, CA 94598

Timed MRM Feature Pack

Varian MS Workstation Version 6.9.3 Service Pack 2
Release/Update Notes

Overview

This document is organized into three broad categories:

- Timed MRM Features
- Items of Interest to All Users of the Varian MS Workstation Version 6.9.3 SP2
- Items of Interest to Users Upgrading from MS Workstation Version 6.9.3 or 6.9.3 SP1

All Varian MS Workstation operators should read the section "Items of Interest to All Users of the Varian MS Workstation Version 6.9.3 SP2."

Customers upgrading from an earlier version should read the other sections, as well as Release Notes documents from previous releases, as appropriate.

Timed MRM Features

MS Workstation 6.9.3 SP2, which contains the timed MRM (tMRM™) Feature Pack, gives users the flexibility to automatically optimize the acquisition segments of a multi-transition MRM method. The optimization can provide improved productivity, peak shape, and sensitivity for a complex multi-transition acquisition method.

The MRM database (LCMS Pesticide DB.xls) is included as part of the 6.9.3 SP2 MS Workstation release. The database provides a spreadsheet of many compounds relevant to pesticide screening that can be used as a starting point for creating a new method. Compound information from this database can be directly imported into the MS Workstation Method Editor by using the tMRM feature.

Please refer to page 13 of these release notes for a detailed description of how to use this feature.

Items of Interest to All Users of the Varian MS Workstation Version 6.9.3 SP2

General Operational Considerations

SYSTEM REQUIREMENTS

Ensure that your computer meets the Minimum Computer Requirements listed below. System performance may be poor if minimum requirements are not met:

- Operating System: XP Professional. Windows 98, Windows 2000, and Windows NT are no longer supported. Windows Vista and 7 are not yet supported.
- Pentium 4 (or higher) processor, at least 3 GHz, or greater.
- Video screen supporting 1280 x 1024 x 256 resolution or greater. 16-bit color is recommended.
- At least 2 GB RAM
- CD-ROM drive, 16X or faster

INSTRUMENTS SUPPORTED

MSWS 6.9.3 SP2 supports the following Varian MS instruments:

- GC/MS: 300-MS, 320-MS, 200-MS, 225-MS, 240-MS/4000, Saturn 2000
- LC/MS: 325-MS, 310-MS, 320-MS, 500-MS

MSWS 6.9.3 SP2 does NOT include drivers for the 430-GC, the 920-LC or the 940-LC models. Support for the 850-MIB is now included, provided it is running with the latest firmware (v2.002). Proper operation of 1200 and 1200L instruments is not validated for MS Workstation versions later than 6.9.1.

ANTI-VIRUS SOFTWARE

System performance in general and quantitation in particular, can be seriously degraded if anti-virus software is enabled or other software running that competes for system resources. While your system will run with these limitations, you will not obtain the optimum performance.

Ideally, anti-virus scanning would only be done at computer boot-up or during low-usage times. If it must be run during regular operation, either disable On-Access Scanning (if corporate policies allow and your network is secure) or, at the very least, only include potentially dangerous file types (such as .EXE, .DLL) in, and exclude the MS Workstation File Type extensions (.XMS, .SMS, .MS, .RUN, .SMP, .RCL, .MTH, .SWT, and especially .TMP.) from, automated scanning by your anti-virus software. Consider also excluding the \VarianWS root directory.

Note that if you run McAfee Enterprise 8.0i, there are serious problems running the MS Workstation (and other software as well), unless “Patch 11” from McAfee is installed. Search for *KB43256* at knowledgemap.nai.com for more information.

WINDOWS POWER SCHEMES AND COMMUNICATION FAILURES

Some of the Power Scheme options that can be selected in Windows may disable the communications devices used to control MS Workstation instruments. Under Start | Control Panel | Power Options, on the Power Schemes tab, please ensure that both *System standby* and *System hibernates* are set to *Never*. If the system goes into standby or if the system hibernates, communications failures may occur and, if an acquisition is occurring, data may be lost.

WINDOWS AUTOMATIC UPDATES AND COMMUNICATION FAILURES

Enabling Automatic Windows updates can lead to automated restarts that can interfere with automation runs. Under Automatic Updates in the Control Panel, it is recommended that the user does not select the “Automatic (Recommended)” option, but instead uses the next option “Download updates for me, but let me choose when to install them”.

USE OF MS ACCESS-BASED TEMPLATES

The Application-specific and Custom Reporting elements are implemented using template files (.MDBs) based on Microsoft Access.

These templates are qualified to work with a run time version of Access 2000, which is installed automatically by the MS Workstation installation program.

If a version of retail Microsoft Office is installed on the target computer, the following conditions apply:

Custom Report templates are only compatible with Retail Access 2000, and not with any other version of Microsoft Access.

If Retail Access 2000 is present, it must have been updated to Service Release 1 (SR-1) or later and have been updated with Service Pack 5 for Jet 4.

If a Retail version of Microsoft Office XP is installed on the target computer after the MS Workstation is installed, it will install Access XP, which is incompatible with these templates. No versions of Access other than the Retail version of Access 2000 described above should be installed after the MS Workstation is installed.

Installing the MS Workstation

BEFORE INSTALLING THE MSWS SOFTWARE

It is advisable to perform common disk maintenance tasks such as basic disk checks, cleanup and defragmentation before getting started with this or any other software installation.

In order to install the software and be in a position to efficiently operate the software, you should start with at least 1 Gigabyte of free space on your hard disk prior to the installation. Operating too close to full disk capacity generally leads to performance problems.

If you plan to install the NIST Library Option, please do so before installing the MS Workstation. Otherwise, the MS Workstation installation will install the demonstration version of the NIST library and MS Search Program.

INSTALLING THE SOFTWARE

MS Workstation Version 6.9.3 SP2 can be installed in one of two ways:

1) A Service Pack Update, which requires that MS Workstation Version 6.9.3 or 6.9.3 SP1 already be installed on the system
2) A full release containing a set of two CDs (Setup and Documentation Disk), which does not require a user to have a previously installed version of MS Workstation on their system

The following information pertains to the user who is installing MS Workstation Version 6.9.3 SP2 from the Setup disk.

Administrator Privileges Required: Since the MS Workstation installs device drivers on your computer, you must be logged into an account with Administrator privileges before attempting to install the software on XP systems.

Warning: Do not use the *Install Program as Other User* feature to select another login. Instead, stop the installation, log out of the non-privileged account and into a privileged account restarting the installation. It is best to make sure that you are running from an Administrator account before you start the installation process.

Getting Started: Insert the *Setup* disk in a CD drive on your computer. An installation program should start automatically (allow a few seconds); if the program does not start automatically, please execute INSTALL.EXE from the root directory of the CD.

Select 'Install', then one or more of the following options as appropriate:

Install PCI GPIB Driver: Choose this option if you need to install one or more GPIB cards for the Saturn 2000 module, or the ProStar 230/240/310/330 Modules. This should be done before installing the rest of the MSWS Software.

Upgrade Ver 5.x to Ver 6.9.3 MSWS: Choose this option if MSWS 5.x is currently installed. You will need to provide an upgrade serial number from the S/N card included in your upgrade kit and serial numbers for the options you need to install. While the serial numbers for most 5.x options (EnviroPro, ToxPro, etc…) can be used with MSWS 6.9.3 SP2, serial numbers from pre-6.5 versions of the core MS Workstation software will not work with 6.9.3 SP2. You must purchase an upgrade to use the MSWS 6.9.3 SP2 software.

Update Ver 6.x to Ver 6.9.3 MSWS: Choose this option if a previous version of MSWS 6.x is installed. The serial numbers will be automatically re-entered. However,

while the serial numbers for most 5.x options (EnviroPro, ToxPro, etc…) can be used with MSWS 6.9.3 SP2, serial numbers from pre-6.5 versions of the core MS Workstation software will not work with 6.9.3 SP2. You must purchase an upgrade to use the MSWS 6.9.3 SP2 software.

Install MSWS Software: Choose this option if no MSWS version is installed. You will need to provide a serial number for the MSWS and any of the options you purchased.

Please review the terms of the licensing agreement. If you reject the agreement, the installation program will exit.

If the installer cannot locate the NIST MS Search program, it will give you the opportunity to install a demo version of the NIST software. This demo version includes the search engine, which will allow you to create and search NIST User Libraries from within the MS WS software, or use other commercial libraries such as Wiley Registry 8th edition.

The Module Driver for the 300-MS, 310-MS, 320-MS, and 325-MS is named "Quad Mass Spec" as it supports multiple models of quadrupole MS modules.

At the end of the installation, turn off the computer and install any interface cards required for your hardware (Quad PCI interface, GPIB boards, etc.) before restarting your computer.

After the installation of the interface cards is complete, proceed to installing the Documentation CD. You can choose to install the manuals on the hard disk, or just access the manuals from the CD.

Note: We recommend you answer 'Yes' when asked if you want to install the manuals.

OPTIONS/SERIAL NUMBERS

The Windows-based installer includes the ability to install many of the optional MS Workstation application programs as part of the core installation; one may simply keep entering product serial numbers into the single installation program to install multiple products rather than launch multiple installers separately.

Upgrades of existing MS Workstation (or Saturn GC/MS Workstation) installations will require that you enter the new serial number that came with your upgrade kit for the core MS Workstation 6.9.3 SP2 software. Optional software such as ToxPro Plus and EnviroPro will not require new serial numbers for upgrades.

MICROSOFT ACCESS

The Access 2000 Runtime is installed automatically as part of the core installation.

NIST MS SEARCH AND AMDIS PROGRAMS

The NISTDEMO Library and MS Search Program are installed automatically if a full version of the NIST Library and MS Search Program is not already installed. If an older version of the MS Search Program is already installed, it will be upgraded to the current version

If an older version of the NISTDEMO is installed, it will be replaced with the latest demo version. This latest version now supports the Varian XMS file types. Note that AMDIS only supports data files with a single Scan Descriptor (aka Scan Channel) per Method Segment. Multi-Channel data files cannot be analyzed.

If an older version of the full NIST Library and MS Search Program is installed, the core Workstation installation will proceed after displaying a message about later updates being available. Please see your Varian representative if you wish to upgrade to the latest full NIST MS Search Program, AMDIS and Libraries.

MS Workstation Operational Considerations

MS Workstation and Network Operation

The Varian MS Workstation allows a single, standalone PC to control a single logical instrument comprising multiple, cooperating modules (e.g., an Autosampler, GC or LC, and Mass Spectrometer). The MS Workstation is not a Client/Server-based system and, consequently, does not support multiple instrument control, simultaneous user connections to one or more instruments, or simultaneous/shared access to a set of Workstation Application Files (Methods, Data files, Sequences, or SampleLists, etc.).

Varian does not recommend or support the use of the MS Workstation for accessing or processing any Workstation Application Files located on a shared storage device, such as a network file system. The MS Workstation assumes dedicated access to all files that it processes and makes no provisions for synchronizing the actions of one user with another. As such, Application and Data File corruption could result; rendering the files so accessed unusable.

Multiple Users On A Single MS Workstation

Note that a file created by a user in a location that is private to this user will – as it should – not be generally accessible to other users. It is therefore recommended that files only be created in a location that is "below" the Workstation folder (c:\varianws by default), or in an area that has been set up to be accessible by all Workstation users by the System Administrator.

Note that the same thing applies to the directories in which NIST and AMDIS are installed. If a particular user is not given write access rights to the files, the software will not work properly.

Concurrent Use of Method Files

In general, a method should not be used in two applications simultaneously. In particular, methods used for automated acquisition and data handling in System Control should not also be open in Method Builder or in MS Data Review.

If the temporary copy of a method that is used in the Results View in MS Data Review is modified and then saved back to the permanent method, you will be warned if the method has been changed in another application. The temporary changes that were made in the Results View then can be saved back to the original method, saved to a new method, or discarded. Saving the changes to the original method will overwrite any changes that were made by the other application, including the compound calibration curves. Changes that were made to the method before the Results View is accessed to view and modify results cannot be prevented. To avoid overwriting the calibration curves that were used to calculate existing results, it is recommended that you save a copy of the method to the directory that contains the data files and process them with that copy.

Quad MS Driver

The Quad MS driver is installed if selected during the installation program. An Icon will appear in the Available Modules area in the configuration screen of System Control whether a Quad MS is present or not. If you do not plan to connect a Quad MS, you can make the icon disappear by disabling the module driver. This can be done by selecting ***Enable/Disable Instrument Modules…*** in the right-click menu of the Workstation ToolBar. System Control must be restarted for this to take effect.

Saturn 2000 and LC Modules

If both the Saturn 2000 and LC Modules are selected for installation, then Saturn 2000 will be installed with data handling capability only. As the Saturn 2000 and

certain LC Modules both use the same GPIB interface, their use is mutually exclusive.

MS DATA REVIEW

Displaying expanded directories in the Plots View Data Files pane that contain large numbers of data files can affect the performance of MS Data Review when the tree display is updated. Automatic display updating is disabled by default. For optimum performance when display updating is done either automatically or manually, directories should not contain more than 1,000 data files. MS Data Review may take significantly longer to open to the Plots View the first time that it is started after installing the software.

Because network access can be slow and sometimes unreliable, quantitation should not be performed on files stored on a network.

Attempting to select some types of corrupt MS data files can cause the MS Data Review application to close. If the Application Start Up Preferences dialog specifies that the Last Recalc File or Last Data File should be auto loaded when the application is started, and if the data file that it tries to load is corrupt, the application will close immediately after starting. If this happens, the simplest way to start MS Data Review is to double-click on a valid file in Windows Explorer.

Known Issues in MSWS 6.9.3 SP2

MS DATA HANDLING

Id: 6673	**Title:**	**MSDR scan descriptors confused by missing driver**
	Area:	MS Data Review
	Descr.:	For some MS models, it may not be possible to form the proper scan descriptors in a data file unless the corresponding driver is installed. When this occurs, the scan descriptors are of the form 'Chan 1.2' meaning Channel 1 in segment 2. We recommend you enable the drivers for all the MS Modules whose data you may need to review.

QUADRUPOLE MS

Id: 5899	**Title:**	**Manually changing operating conditions while automated functions are running can cause them to fail.**
	Area:	Quad: Status & Control Window
	Descr.:	While performing automated functions, such as EDR calibration or Auto Tune, if the user changes the scanning (or other) conditions, the automated function may fail as the data returned might not be what the automated function is expecting. Avoid making such changes while an automated function is running.
Id: 5652	**Title:**	**Running more than one automated function at the same time can cause one or both to fail.**
	Area:	Quad: Status & Control Window
	Descr.:	The Quadrupole software will allow the user to try to initiate and run multiple actions concurrently (and have several dialogs open simultaneously). In general, this can cause problems and should be avoided.

Items of Interest to Users Upgrading from MS Workstation 6.9.3 or 6.9.3 SP1

What's New in MSWS 6.9.3 SP2

The primary purpose of the MS Workstation 6.9.3 SP2 release is to provide support for the Timed MRM Feature Pack, Scan Channel Validation, and control of the 850-MIB in MS Workstation.

What's New in MSWS 6.9.3 SP1

The primary purpose of the MS Workstation 6.9.3 SP1 release was to provide support for the 3.02 Firmware of the 450-GC Module Driver, Manual Integration of Qualifier Ions in MS Data Review, and Improvements in MS Data Review Performance.

The 450-GC Module now supports the 3.02 version of 450-GC Firmware. Customers upgrading to 6.9.3 SP1 who have a 450-GC Firmware version prior to 3.02 will need to upgrade the 450-GC Firmware to Version 3.02 in order to operate the 450-GC in 6.9.3 SP1.

HotFixes included in 6.9.3 SP1/SP2

Id:	Title:	Allow 0 for Cycle Time in PrepAhead
HF 100039	Area:	CombiPal
	Descr.:	The Cycle Time can now be set to 0 for PrepAhead when using SPME or Headspace Injection Modes.

MS Data Handling Changes

ENHANCEMENTS IN MSWS 6.9.3 SP2

Accumulate Changes before Reprocessing

It is now possible to make multiple Peak Event or Time Event changes on a particular compound without having to reprocess each individual change. For example, the user can now make multiple manual integration changes on a compound on multiple files in a recalc list without having to wait for the entire recalc list to be reprocessed after each manual integration change.

This feature can be enabled or disabled through the Results View Preferences. The Default setting is set to Accumulate Changes.

Dedicated Directory for Temp Files

A new folder has been created in the C:\VarianWS directory called WSTemp. This folder contains all the *.tmp files that are created during the use of MS Data Review. This separate folder can now be easily excluded from Anti-Virus Scanning, which will help in the speed of data file processing within MS Data Review.

MS/MS Library Search Improvements

1) The Precursor Ion and spectra are now exported to the *.msp file so that MS/MS Library Searching can be performed using the NIST MS Program. The user must manually export the file to *.msp and then perform the search from with-in the NIST Library Search Program. The integrated library search (NIST icon) does not currently support the MS/MS library searching.
2) Spectral Averaging is no longer restricted on MS/MS and DDS spectra in MS DataReview.

Tuning Report Annotation Improvement (EnviroPro)

The scan number and retention time of the best tune has been added to the Tune Report in Envirpro.

NEW FEATURES IN MSWS 6.9.3 SP1 AND LATER

Manual Integration of Qualifier Ions

Manual Integration of Qualifier Ions is now available when the "Qualifier Integration" option is set to "Quan Ion Pts" and the "Report Outliers as" option is set to "Failed" in the Calculations Set-up dialog of the Method Editor. It is NOT available when the Qualifier Integration is set to "Independent" or if the "Report Outliers as" field is set to Missing, even if Quan Ion Pts is specified. When files are processed, Qualifier Ions can be manually integrated in the same way that users have previously been able to manually integrate the Quan Ion.

There are some features that the user should be aware of when doing manual integration of qualifier ions:

1) After a Manual Integration event has occurred on a Qualifier Ion, a "q" will be displayed when "Status" is selected in the Reports section in the method editor or in the Results List Preferences in the Results View, to indicate that a Qualifier Ion has been manually integrated. If a compound has more than one Qualifier Ion, "q" will be displayed only once, even if all the Qualifier Ions for that compound have been manually integrated.

2) Restore Start/End Points will put the Integration Event marker back to the original Start/End Points as determined by the Method Processing.

3) Changes to Method Parameters will result in any Manual Integration Events being cleared for the currently selected compound. Method Parameter changes include changes made through the "Edit" button and changes to Time Events.

4) Click and Drag Integration is available for Qualifier Ions. This feature can be accessed through the "Set Click and Drag Action" drop down option of "Integrate Area" or just holding down the "I" key while moving the cursor over the desired area of the chromatogram. In order to restore the original start conditions, the user must discard the changes, through the "Save/Discard" button. Clicking on the "Save/Discard" button will provide the option to discard the click and drag changes. This will discard all changes that have been made since the previous Save action.

5) If a processed compound is Missing, then there will be no Integration Event Markers on the Qualifier Ions. If the user manually integrates the Quan Ion so that the compound is no longer missing, the qualifier ions will be integrated automatically. The qualifier ion results then can be manually integrated, if desired.

6) Since Qualifier Ion Ratios are only used to confirm the identification of a compound, manual integration of a Qualifier Ion result for a compound does not affect Quan Ion integration, quantitation results, or the corresponding calibration curve. In addition, including points, excluding points, or changing calibration curve parameters from a compound calibration curve does not affect any existing Qualifier manual integration results for the compound.

7) When Method Parameters are edited, either through the Edit button or the Time Events bar, in the Results View, the user will be prompted with a warning that all Manual Integration events will be cleared for that compound. The user can select to have the warning displayed every time a Method Parameter change has occurred or disable the warning. If the user decides to disable the warning message, it can easily be restored. To Restore the warning message, click on the Preferences Menu Item and select the "Restore Disabled Warnings" option.

ENHANCEMENTS IN MSWS 6.9.3 SP1 AND LATER

Performance Improvements in Process and Results Views

In MS Workstation Version, 6.9.3 SP1, the speed of processing files and displaying and modifying results has been improved. The results presented below show one example of the improvements over past versions of the Software.

Note: All users may not see the exact same improvements because selected method parameters, file size, and virus-scanning will affect performance of MS Data Review actions.

The first table below provides basic information about the method and data files used to compare performance. The second table illustrates the performance improvements seen between MS Workstation Version 6.9.3 and MS Workstation Version 6.9.3 SP1:

General Information about Method/Data files used in Performance Tests

Instrument	Triple Quadrupole MS
Size of Data Files	~ 85 MB
Number of Data Files in Recalc List	8
Data File Type in Recalc List	Analysis
Number of Time Segments in Method	6
Number Transitions in Method	585
Number of Compounds in Compound Table	251
Library Search Unknown Peaks	Disabled
Report Unknown Peaks	Disabled
Qualifier Integration	Independent
Display Preferences in Results View	Recalc List Sort Order: Peak Name Retention Time (min)

Improvements in 6.9.3 SP1 vs. 6.9.3

Action	Improvement in 6.9.3 SP1 (x factor)
Process Recalc List (Process View)	2
Results View Actions:	
1st time Manual Integration	5
Subsequent Manual Integration	5

1st Time Edit Method Parameters (Edit Button)	3
Subsequent Edit Method Parameters (Edit Button)	6
1st Time Adding Time Event	3
Subsequent Time Event Changes	5
Create Compound Reports: All	2

Changes to the Edit Button

If the user displays the Method Parameters dialog by clicking on the Edit button from within Results View of MS Data Review, makes no changes, and clicks on Ok instead of Cancel, the files will not be reprocessed. Previously they were reprocessed, which could result in a significant delay.

General Guidelines

Below are some general guidelines for optimizing speed performance in MS Data Review, which affect all users of MS Workstation. The method parameter guidelines should be followed whenever they are appropriate for the data that is being acquired.

Computer Settings:

1) Computers should meet the current MS Workstation hardware specifications. In particular, at least 2 GB of RAM should be installed.
2) Disable auto-scanning by Anti-Virus Software of the VarianWS Directory and *.tmp files. If it is not possible to disable entire folders, disable the following file types: *.tmp, *.xms, *.sms, *.ms, *.run, *.smp, *.rcl, *.mth, *.swt, and *.mdb.
3) When processing data files, make sure that the data files are on a local PC and not on a network. If directories are excluded from anti-virus scanning but file types other than .tmp are not, make sure that the data files are under the VarianWS directory.
4) If appropriate, display the Results List pane by compound, not by recalc list

Method Parameters:

5) Use Quan Ion Pts for Qualifier Integration. For example, in MS Workstation Version 6.9.3 SP1, selecting Quan Ion Pts instead of Independent for Qualifier Integration results in a 1.5x performance enhancement during data processing. In addition to being significantly faster than Independent integration, the qualifier results can be manually integrated.
6) If Spectrum Matching is not required for reliable compound identification, use RT Identification.
7) Use smaller Search Windows. They must be large enough to contain the apex of the integrated peak of interest in all data files that are processed.
8) If not needed, disable Library Searching of Unknown Peaks and disable Report Unknown Peaks
9) If library searching is done, set the Reporting Threshold to only report the unknown peaks of interest. Only these peaks will be searched.

Triple Quadrupole MS systems

For new users of MS Workstation or current users setting up new methods, the best way to increase quantitation speed of data files and recalc lists is to use the suggestions below as guidelines for reducing file size:

1) Use as many time segments as possible, while minimizing the number of compounds that may cross segment boundaries
2) Reduce the number of MSMS transitions per segment

If the user is able to do items 1) and 2), then the dwell time for each transition over all segments will be significantly increased and there will be a reduction of the scan time in each segment.

The user can expect to see the following changes if methods are set-up in this manner:

1) Decrease in overall file size, which will speedup quantitation
2) Increase in the number of data points over each chromatographic peak, which provides better peak integration.
3) Spectral quality is improved by the longer dwell times.

Quadrupole MS Module Changes (300-MS/310-MS/320-MS/325-MS)

ENHANCEMENTS IN MSWS 6.9.3 SP2

Scan Channel Validation

Previously, a patch was available to address a problem regarding transitions in the compound table becoming out of sync with the corresponding compounds in the acquisition method when transitions were deleted or added to the method. This patch has been incorporated into the MS Workstation 6.9.3 SP2 Release. A preference is located in the General Preferences Section of MS DataReview, which enables/disables the Scan Channel Validation. This preference eliminates the need for the patch that has been available since 2007.

When the Validate Scan Function Preference is enabled (MS Data Review → General Preferences → Validation), the following items will be observed:

1) The scan channel specifications for all compounds will be correct in the compound table after transitions are added or deleted in the acquisition method.
2) Compound retention times will be automatically updated in the compound table if segment acquisition times are changed.
3) If a selected compound contains a deleted transition, the user will be warned and the missing scan function channel will be labeled as “255” in the Compound Table. Processing a compound with an invalid scan function channel will result in a warning and the compound will not be quantitated.

Note: While Scan Channel Validation works for both deleting/adding transitions to the Acquisition Method and for when segment times have changed, the user cannot change both the number of transitions and segment times at the same time. For example, the user can add/delete transitions to the Acquisition Method, but must open the compound table BEFORE changing the segment times in the Acquisition Method. Similarly, the segment times can be changed in the Acquisition Method, but the compound table must be opened BEFORE the user can add/delete transitions in the Acquisition Method.

If users do not wish to use the Scan Channel Validation, it can be disabled through the General Preferences of MS DataReview. The compound table can be manually fixed if Scan Channel Validation is Disabled or if the acquisition method and compound table are already inconsistent before enabling the Scan Channel Validation by performing the following steps:

1) Acquire a data file with the modified acquisition method.
2) In the Data Handling Method Editor, select the new data file.
3) Go to the Quan Ions page in the compound table for each compound that is affected, and re-select the desired transition(s) from the list of available transitions.
4) Save the method.

Note that the acquisition method that was used to create a data file can be extracted from it, so the method can always be re-created if the original method was later modified or no longer exists.

Timed MRM (tMRM)

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

A brief description of how to use the tMRM tool is found below. A full description can be found in the Software Operation Manual of the 320-MS and 325-MS Manuals.

1) To open the tMRM tool, click on the Schedule tMRM button from the Quad Acquisition Method Section.
2) To create a spreadsheet that is compatible with the tMRM tool:
   a) Click on the "Make Template" button, which will prompt the user to save a template in the correct *.txt format.
   b) To export transitions from an existing method, click on "Export" button after selecting the correct method.
   c) Use the MRM database (LCMS Pesticide DB.xls) to select transitions. Instructions are included with-in the spreadsheet for selecting compounds.
3) Add MRMs to the Spreadsheet:
   a) Open the tMRM Spreadsheet in Excel® and fill in the missing data for each transition. The following fields must contain data: Polarity (+/-), Q1 First Mass, Q3 First Mass, Capillary, Collision Energy, Dwell Factor, Retention Time, and Retention Time Window. The CAS Number, Compound Name, Q1 Last Mass, and Q3 Last Mass are not required fields.
   b) Save the spreadsheet as a tab-delimited text file.
4) Import MRMs to the Scan Method from the Spreadsheet:
   a) Select the input spreadsheet name in the "Import MRMs to Scan Method" Filename box.
   b) Specify Requested Scan Time or Requested Dwell Time (the Dwell Factor from the spreadsheet will be used in conjunction with these specifications to weight the actual dwell time used for each compound), the minimum segment time width, and the maximum number of time segments to be used.

      Note: If the tMRM parameters are not chosen to accommodate all of the transitions in the spreadsheet, transitions may not be imported into the method.
   c) Click on Import to schedule the timed MRMs. The Import Statistics will be updated each time a new spreadsheet is imported.

CORRECTIONS IN MSWS 6.9.3 SP1 AND LATER

Id:	Title:	Quad Ms tune reports use mass cal from active scan method
6913	Area:	3X0-MS – Autotune Reports
	Descr.:	A correction was made to ensure that when "Report Only" is selected in AutoTune, the mass peak widths of Q1 and Q3 that are used to generate the report are set to calibrated, regardless of what is specified in the Active Scan Method. After the report is generated, the mass peak width will be returned to its previous value.

450-GC Module Changes

ENHANCEMENTS IN MSWS 6.9.3 SP1 AND LATER

MS Workstation Version 6.9.3 SP1 now supports 450-GC Firmware Version 3.02.

The following changes have been made to the Method Editor of the 450-GC in order to accommodate changes made to Firmware Version 3.02:

1) The Sample Delivery Table of the Method Editor will now only accept 30 lines.
2) It is now possible to Enable/Disable the Flow/Pressure and Detector EFCs on the 450-GC. The Method Editor has been updated to reflect this change.

CORRECTIONS IN MSWS 6.9.3 SP1 AND LATER

Id: 6912	**Title:**	Sample List Report Prints wrong injection volume
	Area:	GC Module – Sample LIst
	Descr.:	For sample lists created with a 8400/8410 and a 450-GC, the Injection Volume was previously being printed incorrectly on the Sample List Report. This defect has been resolved in the current software release.

StarWriter Changes

CORRECTIONS IN MSWS 6.9.3 SP2

A crash that occurred when opening 450-GC files in the chromatogram object has been corrected.

8XX-MIB Module Changes

ENHANCEMENTS IN MSWS 6.9.3 SP2

The MSWS now supports the 850-MIB, assuming it is running the latest firmware (v2.002). Only the two-channel ADC configuration (03-950205-11) of the 850-MIB is supported. In addition, different from the 800-MIB, the 850-MIB can only be used with a Fixed IP Address. Currently there is no means through MSWS to assign a Fixed IP address to the 850. A Field Service Representative will need to set the 850-MIB IP Address using the Galaxie Configuration Manager.

CombiPal Module Changes

CORRECTIONS IN MSWS 6.9.3 SP2

While operating in Headspace mode, a timing problem that would cause missed injections has been corrected.