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

Varian MS Workstation Version 6.9.1 Release/Update Notes

Overview	2	Items of Interest to Users Upgrading from MS Workstation 6.9	8
Items of Interest to All Users of the Varian MS Workstation Version 6.9.1	2	What's New in MSWS 6.9.1	8
General Operational Considerations	2	Core Workstation Platform	8
System Requirements	2	New Components in MSWS 6.9.1	8
Instruments supported.....	2	Corrections in MSWS 6.9.1	8
Anti-Virus Software	2	Corrections in MSWS 6.9 SP2	8
Windows Power Schemes and Communication Failures	3	Corrections in MSWS 6.9 SP1:.....	9
Use of MS Access-based Templates	3	2000 GC/MS Ion Trap Module Changes.....	9
Installing the MS Workstation	3	4000 GC/MS Ion Trap Module Changes.....	9
Before Installing the MSWS Software	3	General Information	9
Installing the Software	3	Corrections in MSWS 6.9.1	10
Options/Serial Numbers.....	4	Corrections in MSWS 6.9 SP1	10
Microsoft Access.....	4	500 LC/MS Ion Trap Module Changes	11
NIST MS Search and AMDIS Programs.....	4	Corrections in MSWS 6.9.1	11
MS Workstation Operational Considerations	5	MS Data Handling Changes	11
MS Workstation and Network Operation	5	Improvements in MSWS 6.9.1	11
Multiple Users On A Single MS Workstation	5	Corrections in MSWS 6.9.1	11
Concurrent Use of Method Files.....	5	Corrections in MSWS 6.9 SP2	12
Quad MS Driver	6	Corrections in MSWS 6.9 SP1	13
Saturn 2000 and LC Modules.....	6	Quadrupole MS Module Changes (1200/1200L/300-MS/310-MS/320-MS)	14
MS Data Review	6	General Information	14
Known Issues in MSWS 6.9.1	6	Improvements in MSWS 6.9.1	14
450-GC	6	Corrections in MSWS 6.9.1	14
MS Data Handling.....	7	Corrections in MSWS 6.9 SP2	14
Quadrupole MS.....	7	Corrections in MSWS 6.9 SP1	17

Overview

These Release Notes are organized into two broad categories:

- Items of Interest to All Users of the Varian MS Workstation Version 6.9.1
- Items of Interest to Users Upgrading from MS Workstation Version 6.9

All Varian MS Workstation operators should read the section “Items of Interest to All Users of the Varian MS Workstation Version 6.9.1.”

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

Items of Interest to All Users of the Varian MS Workstation Version 6.9.1

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: Windows 2000 or XP Professional. Windows 98 and Windows NT are no longer supported. Windows Vista is not yet supported.
- Pentium III (or higher) processor, at least 1 GHz, or greater.
- Video screen supporting 1280 x 1024 x 256 resolution or greater. 16-bit color is recommended.
- At least 1GB RAM
- CD-ROM drive, 16X or faster

INSTRUMENTS SUPPORTED

MSWS 6.9.1 supports the following Varian MS instruments:

- GC/MS: 300-MS, 320-MS, 200-MS, 240-MS/4000, Saturn 2000, 1200, 1200L
- LC/MS: 310-MS, 320-MS, 1200L, 500-MS

In addition to a variety of GC and LC modules, MSWS 6.9.1 introduces drivers for the new 450-GC and 431-GC models. MSWS 6.9.1 does NOT include drivers for the 430-GC, the 920-LC or the 940-LC models.

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 knowledge.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.

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

Since the MSWS Workstation installs device drivers on your computer, you must be logged into an account with Administrator privileges before attempting to install the software on Windows 2000 or XP systems. (In particular, do not use the *Install Program as Other User* feature. First log out of the non-privileged account and into a privileged account before completing the installation.)

Insert the distribution 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 6.9.1 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 6.9.1, serial numbers from pre-6.5 versions of the core MS Workstation software will not work with 6.9.1. You must purchase an upgrade to use the MSWS 6.5 (or later) software.

Update Ver 6.x to Ver 6.9.1 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 6.9.1, serial numbers from pre-6.5 versions of the core MS Workstation software will not work with 6.9.1. You must purchase an upgrade to use the MSWS 6.5 (or later) 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 ask you to provide the location of the NIST program. You can use 'Cancel' to indicate that the NIST software is not installed, in which case a demo version will be installed. This demo version includes the search engine, which will allow you to create and search NIST User Libraries from within the MS WS software.

The Module Driver for the 1200, 1200L, 300-MS, 310-MS, and 320-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.

OPTIONS/SERIAL NUMBERS

The Windows based installer includes the ability to install 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 6.9.1 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 a 1.7 version of the MS Search Program is already installed, it will be upgraded to Version 2.0a.

If an older version of the NISTDEMO is installed, it will be replaced with the latest demo version. This latest version includes version 2.64 of AMDIS which 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, 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 the 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 6.9.1

450-GC

GC Status in Setup Ethernet Communications dialog

In the Setup Ethernet Communications dialog in System Control, the status of a properly operated 450-GC may be improperly reported as 'In Use By <unknown>' or 'Not responding'.

'In Use By <unknown>' is observed when the GC is in the same subnet as the controller PC.

'Not responding' may be observed when the GC is in another subnet.

In both cases, the problem does not affect the operation of the GC. The root cause of the problem will be corrected at the earliest opportunity in the GC firmware.

Lower Temperature Limit for Column Oven, 1079, 1093, and SPT

The method editor for the 450-GC driver will accept temperatures down to -99°C regardless of the cooling option installed. The temperature limits accepted by the GC for the Column Oven and the 1079, 1093, and SPT injectors are as follows:

Coolant	Lower Temp Limit
LN2	-100°C
LCO2	-60°C
Air / No Coolant	+20°C

Methods requesting values lower than the limit appropriate for the installed option for each component will fail to activate, make sure your methods specify limits appropriate for the coolants used.

MS DATA HANDLING

When a transition is added to (or deleted from) a Quadrupole Acquisition Method Time Segment, it changes the physical channel for other transitions in the segment that have a higher Precursor mass. This will invalidate any existing compound table specifications in the data handling method that reference these transitions. This problem will be addressed in a future release; a preliminary patch for this specific issue is available on request.

To fix the compound table in the current software:

1. Acquire a data file with the new 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 you can now easily extract the original acquisition method from each data file, so you can always recreate the original method if the file was later modified or no longer exists.

Id: 6673	<p>Title: MSDR scan descriptors confused by missing driver</p> <p>Area: MS Data Review</p> <p>Descr.: For some MS models, it may not be possible to form a proper scan descriptor for a channel of 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 whose data you may need to review.</p>
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QUADRUPOLE MS

Id: 5899	<p>Title: Manually changing operating conditions while automated functions are running can cause them to fail.</p> <p>Area: Quad: Status & Control Window</p> <p>Descr.: While performing automated functions, such as EDR calibration or Auto Tune, if the user changes the scanning (or other) conditions that 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.</p>
Id: 5652	<p>Title: Running more than one automated function at the same time can cause one or both to fail.</p> <p>Area: Quad: Status & Control Window</p> <p>Descr.: The Quadrupole software will currently 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.</p>

Items of Interest to Users Upgrading from MS Workstation 6.9

What's New in MSWS 6.9.1

The primary purpose of the MS Workstation 6.9.1 release is to provide drivers for the new 200-MS, 431-GC and 450-GC modules.

Additional improvements and corrections to Module Drivers, MS Data Handling and MS Data Review have also been included.

MSWS 6.9.1 includes all of the changes and improvements implemented in MSWS 6.9 SP1 and SP2.

Core Workstation Platform

NEW COMPONENTS IN MSWS 6.9.1

The 200-MS, 450-GC, and 431-GC are new instrument modules with new drivers. As they are closely related to the existing 2000 MS, 3800 GC and 3900 GC, and methods developed on any of the latter modules are applicable to the newer modules. A batch conversion program has been developed to facilitate the conversion of such methods.

2000 MS ↔ 200-MS (bidirectional)

3900 MS ↔ 431-GC (bidirectional)

3800 GC → 450-GC (unidirectional)

The **Method Batch Conversion** program can be found under the

Start->Programs->MS Workstation->Utilities menu. Press the 'Hints...' button in the program's main window to get directions.

Because the 240-MS is handled by the same driver as the 4000 MS and considered to be a newer version of the same module, now referred to as 240-MS/4000, there is no conversion required between a 240-MS and 4000 MS.

CORRECTIONS IN MSWS 6.9.1

Id: 6653	Title: CombiPAL: Invalid Temp values displayed Area: CombiPAL Autosampler Driver Descr.: Under some conditions, large temperature values were displayed on the CombiPAL Status and Control screen in System Control for items that were not installed or not used. These fields now display 'N/A' when appropriate.
Id: 6668	Title: Activating a method in System control (reprocessing only) causes exception Area: System Control Descr.: Activating a method interactively in a 'Reprocessing only' installation crashed System Control. This was corrected in MSWS 6.9.1.

CORRECTIONS IN MSWS 6.9 SP2

Id: 5927	Title: Inject Single Sample makes two injections (& repeated sample list) Area: System Control - Automation Descr.: Under some conditions, a sample list or single sample injection ran twice without any operator action. A potential cause of this problem was corrected
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Id: 6386	Title: 212-LC: Method Printout does not show composition or flow. Area: 212-LC Driver Descr.: Method printouts for the 212-LC did not show composition or flow. Run Log printing/formatting was fine. The problem was corrected in the 212-LC driver.
Id: 6400	Title: CPAL: Automix "Aspirate" command does not work Area: CombiPAL AutoSampler Descr.: The AutoMix "Aspirate" command moves the head to the specify vial, but the needle does not go in the vial. The command was corrected to use the penetration specified in the method.

CORRECTIONS IN MSWS 6.9 SP1:

Id: 5926	Title: Module Information Editor does not work unless .Net is installed Area: Core Workstation Platform Descr.: The Module Information Editor unnecessarily relied on the .Net environment. The module information can now be edited whether .Net is installed or not.
Id: 6046	Title: 3800 issue with 1093 method Area: GC Module driver Descr.: If a 3800 GC was equipped with a 1093 injector, the mechanism updating a newly created method to make it compatible with the on-line instrument configuration failed to properly initialize the 1093 parameters. As a result, the method failed to download, reporting 'Error 4'. The driver was modified to properly initialize the 1093 parameters when making the method compatible with the installed hardware.problem.

2000 GC/MS Ion Trap Module Changes

In MSWS 6.9.1, the default 'q' value in the 'q' Calculators was changed from 0.400 to 0.334. The same applies to the new 200-MS module.

4000 GC/MS Ion Trap Module Changes

GENERAL INFORMATION

Improved Isolation Waveform

A new Isolation Waveform provides a finer isolation, in particular for unstable ions.

Customers who upgrade from older versions to the 6.9.1 release should re-tune their MSMS/AMD/MRM/MSn/uSIS methods for the new values to synergize with the new improved Isolation waveform. The parameters that may require adjustment are the High Mass Ejection Voltage and the Isolation Window. In 6.9.1, these 2 parameters have new default values to reflect the higher efficiency of the new Isolation Waveform.

The new default Isolation Window is 3 Daltons for EI-MSMS and 5 Daltons for CI-MS/MS and Hybrid modes.

The new default value for the High Mass Ejection Voltage has been changed to 12 Volts for EI-MSMS and 8 Volts for CI-MSMS and Hybrid modes.

Pre-6.9.1 methods using the old default values for the High Mass Ejection voltage will be updated when loaded in the method editor.

Acquisition Method Changes

The Acquisition Method format has been changed from previous versions to support new capability. Although methods from previous versions of the software will be converted automatically to the new format when opened with this version, methods from this version of the software cannot be used with earlier releases of the software.

Low Mass Enhancement

A checkbox was added to the Manual Control tab of the Status and Control Window for the 240-MS/4000 module to enable a new **Low mass enhancement** feature. After activating this feature, mass calibration should be performed.

The point of this feature is to increase the sensitivity of the detection of low mass ions (<100 *m/z*), especially for EPA method 521. Use this option only when analyzing masses below 200 *m/z*. Using this feature lowers the dipole voltages for the scan function, and may cause incorrect mass assignment for mass fragments greater than 200 *m/z*.

The status of this feature is documented in the module attributes section of the run log.

CORRECTIONS IN MSWS 6.9.1

Id: 5979	Title: Module Attributes in Run Log have Today's Date/Time in first line Area: MS Data Review - Reports Descr.: The first line of the module attributes contained the current date and time, which was confusing. The date and time were removed from this line. The data and time of the tune are available later in the same report.
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CORRECTIONS IN MSWS 6.9 SP1

Id: 6211	Title: ToxPro Tune Report Does Not Display Air and Water Results for 4000 Data File Area: 4000 – Custom MS Reports Descr.: When a ToxPro FC-43 Tune Report is created from a 4000 MS data file, the Air Level Test and Water Level Test results are not shown as they are on 2000 MS data files. This information is now reported.
Id: 6230	Title: 4000: A burned out filament does not stop automation Area: 4000 Driver - System Control - Automation Descr.: When running automations with a 4000, if the selected filament burns out during a run, a message is logged: "Filament n is not OK", but the automations continue after this point. This error will now stop the automation.
Id: 6312	Title: Loss of CI MS/MS sensitivity when multiple channels are present Area: 4000 Driver - Acquisition Descr.: CI/MSMS sensitivity is not affected in channels after the first channel when multiple compounds are monitored in the same segment.
Id: 6286	Title: Autotune Logs are not created after a clean installation Area: 4000 / 500-MS Drivers - Installation Descr.: In a clean installation, the "VarianWS\Autotune Logs" directory is not created and this prevents the autotune logs from being saved. The directory is now created for new installations.

500 LC/MS Ion Trap Module Changes

CORRECTIONS IN MSWS 6.9.1

Id: 6245	Title: Comments section rewritten when import different include/exclude list Area: 500-MS Control Method Descr.: Only the spreadsheet section of the include and exclude lists are updated when these lists are imported.
Id: 6243	Title: "Load Required for Ready" is not checked as Default Area: 500-MS Control Method Descr.: In Method Builder, Special Applications, the "Load required for Ready" is now checked by default.

MS Data Handling Changes

IMPROVEMENTS IN MSWS 6.9.1

Method extraction from data files

A popup menu was added to the Export button in the Data File Information dialog, with two commands "Export to ASCII" and "Export extracted method".

"Export to ASCII" saves the contents of the list box into a text file (the previous functionality of the Export button).

"Export extracted method" creates a method with all the control and post-run application methods currently in the data file.

CORRECTIONS IN MSWS 6.9.1

Id: 6584	Title: Air Flow scaling causes wrong results when reprocessing in MSDR Results View Area: MS Data Review – Quan, Review Results Descr.: If the Scale Air Flow Samples is specified in the data handling method, reprocessing in Results View caused the wrong Multiplier Value to be displayed in the Results List. This has been fixed so that the correct Multiplier is displayed after reprocessing the results.
Id: 6533	Title: Spectral Averaging problems with decimal mass assignments Area: MS Data Review – Spectrum Edit Descr.: Spectral averaging was not being performed correctly when the spectra to be averaged had masses that differed significantly for the same ion. The calculation for spectral averaging has been corrected in this release.
Id: 6444	Title: Compounds sometimes not identified across segment breaks Area: MS Workstation Platform – Quan Compound Identification Descr.: Compound identification by Spectrum Match could fail if the peak was not in the same data file segment as the target retention time in the method, and if the compound scan function was on different channels in the segments. This was corrected in this release.

Id: 6427	Title: Channels are being swapped when processing across segment Area: MS Data Review – Quan Compound Integration. Descr.: The wrong chromatogram could be generated for compound quantitation if the peak was not in the same data file segment as the target retention time in the method, and if the compound scan function was on different channels in the segments. This could result in the compound being incorrectly reported as Missing or integrated incorrectly, and the displayed chromatogram and spectrum plots could be wrong. This problem was resolved at the same time as #6349 and #6444.
Id: 6349	Title: Ion ratios can fail if Method RT & Peak RT in different segments Area: MS Workstation Platform – Quan Compound Identification Descr.: The confirmation of compound identification by Ion Ratios could fail if the peak was not in the same data file segment as the target retention time in the method, and if the compound scan function was on different channels in the segments. This problem was resolved at the same time as #6427 and #6444.
Id: 6273	Title: DDS: Don't show Difference spectrum in Precursor Ion Path display Area: MS Data Review - TurboDDS Descr.: When the Precursor Ion Path display is selected, the Difference spectrum is no longer displayed for the lowest-level spectrum, even if "Show Difference Spectrum" is selected in the Preferences dialog.
Id: 6171	Title: Change "IS Deviation" to "IS % Dev" Area: MS Data Review – Results List Descr.: The "IS Deviation" column header text in the Results List pane has been changed to "IS % Dev".
Id: 6151	Title: Can't move Quick Integration area labels on plot Area: MS Data Review - MultiChro Display Descr.: Quick Integration Labels and Click-and Drag integration labels can now be moved within MS Data Review's Chromatogram window.

CORRECTIONS IN MSWS 6.9 SP2

Id: 6393	Title: Long Sample ID name can crash Method Builder in Print Preview Area: Data Handling Method MS – Standard MS Reports Descr.: Method Builder can crash when Print Preview is selected if Sample ID is selected as the 'Sort By' key in the Standard MS Reports "Summary Report Format" dialog, and the Sample ID string is very long.
Id: 6366	Title: Ion Time shown for Quad files Area: MS Data Review Descr.: When Quad spectra are displayed, "N/A" is displayed for Ion Time values in spectrum Plot Titles.
Id: 6359	Title: Manual integration sometimes updates calibration replicates incorrectly Area: MS Data Review – Quan, Review Results Descr.: When manual integration changes a compound result from Missing to Identified or from Identified to Missing, the calibration data point replicates sometimes can be updated incorrectly. If the modified calibration point was an Internal Standard, the relative response factors in the data file for all of the compounds that are calibrated with it will be updated incorrectly.

CORRECTIONS IN MSWS 6.9 SP1

<p>Id: 5341</p>	<p>Title: Changing Scan Method invalidates DH Cmpd Table</p> <p>Area: Data Handling Method MS - Compound Table</p> <p>Descr.: When transitions are added or deleted in an acquisition method segment and a compound table already exists in the data handling method, compound specifications for scan functions that are after the added or deleted transitions in a segment will be invalidated. To correct the problem, a data file that has been generated with the modified method must be selected in the method editor, and the correct scan functions must be manually re-selected in the compound table.</p> <p>The compound table scan function specifications should be updated automatically when the physical channel that a transition is specified on is changed. Similarly, data files whose scan function data were collected on different physical channels than what is specified in the method should be quantitated correctly.</p> <p>Note: This fix is not enabled by default. Please contact a Varian representative for more information about this issue.</p>
<p>Id: 6287</p>	<p>Title: MSDR: Select Files dialog only loads first file</p> <p>Area: MS Data Review</p> <p>Descr.: Multiple files can be selected in the MSDR Select Files dialog, but only the first file will be loaded into the Plots View unless the Control key is held down while the Open File(s) button is clicked.</p> <p>All of the files that are selected in the dialog are now loaded without having to hold down the Ctrl key.</p>
<p>Id: 6288</p>	<p>Title: MSDR: Select Files dialog loads TIC even if not selected</p> <p>Area: MS Data Review</p> <p>Descr.: When scan-function chromatograms are specified in the MSDR Select Files dialog for a data file, the TIC chromatogram is no longer displayed in the Plots View if it was not specified in the dialog.</p>
<p>Id: 6300</p>	<p>Title: Using “Move Chromatogram” on a .RUN file crashes MSDR</p> <p>Area: MS Data Review - MultiChro Display</p> <p>Descr.: Using the “Move Chromatogram” function when selecting a .run file will work as expected.</p>
<p>Id: 6303</p>	<p>Title: MSDR: Can’t select file via File Name field in Select Files dialog</p> <p>Area: MS Data Review - Chromatogram Selection</p> <p>Descr.: When a file is selected from the available list in the File Name field in the Select Files dialog, it is not added to the “selected plots” table, its preview file information is not displayed, and it is not loaded into the Plots View when the dialog is closed. It doesn’t matter whether any characters have been typed into the field first to filter the displayed list of available files.</p> <p>Selection, and opening of a file in the Select Files dialog will work as expected.</p>
<p>Id: 6308</p>	<p>Title: DDS: Provide option to display Base Peak Intensity in chromatograms</p> <p>Area: MSDataRev - MultiChro Display</p> <p>Descr.: The ability to display either RIC or Base Peak chromatograms for DDS data files as been added. Users can easily toggle the chromatogram display between Base Peak and RIC.</p>

Quadrupole MS Module Changes (1200/1200L/300-MS/310-MS/320-MS)

GENERAL INFORMATION

Acquisition Method Changes

The Acquisition Method format has been changed from previous versions to support new capability. Although methods from previous versions of the software will be converted automatically to the new format when opened with this version, methods from this version of the software cannot be used with earlier releases of the software.

IMPROVEMENTS IN MSWS 6.9.1

- **Quad model compatibility Check**
When the user requests a change in Quad model type a hardware compatibility check is performed to validate the model switch in the configuration dialog box.
- **Syringe pump off at the end of EDR**
The syringe pump is automatically turned off at the end of the EDR Calibration. Previously, the syringe remained on until the operator acknowledged the successful calibration.
- **CID Calibration**
 - 1) Collision cell zeroing on the 1200L and for the 300 Series MS can now only be performed if there is sufficient vacuum.
 - 2) CID calibration can only be performed if the collision cell zeroing is successful.
 - 3) The CID calibration routine was enhanced by removing potential sources of noise during the calibration.
 - 4) The CID-Ready state is now determined using the flow controller (readback 98) rather than at the convectron gauge (readback 56). This prevents the instrument from being held in a Not-Ready state due to the slower-reacting convectron gauge. Due to the slower response of the convectron gauge, the pressure displayed in the Instrument Status screen may not be the setpoint when acquisition begins, however the pressure in the collision cell has reached the correct value.
- **Tune file loaded automatically at the end of “Tune to Target”**
When the user selects to save the tune file after completion of tune-to-target, the system will now automatically load the tune file at the end of the tune process, similar to the operation of the standard autotune.

CORRECTIONS IN MSWS 6.9.1

Id: 6568	Title: Calibrate "Calibrate All" in EI mode Area: 3X0-MS - System Control Descr.: "Calibrate All" now only calibrates gases that are relevant in the current ion mode. Previously it attempted all calibrations, which caused errors in EI mode.
Id: 6422	Title: Global CID gas value doesn't show up in the run log. Area: 3X0-MS - System Control - Automation Descr.: Added documentation of the global parameters (not segment-based) to the run log.

CORRECTIONS IN MSWS 6.9 SP2

Id:	Title: Mass shift on Q1
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6489	Area: Quad - System Control Descr.: An error was corrected that caused a mass shift in Q1 if a collision cell energy was 0.00 in Full Scan.
Id: 6478	Title: Autotune vs. Report Only flags are inconsistent Area: Quad - Status & Control Window – Auto Tune Descr.: The Autotune report will flag ions that were not used in the tune as “report only, not tuned.” Inconsistencies in the report messages were corrected.
Id: 6477	Title: Air/Water Check runs even when masses 18 & 28 are not tuned. Area: 3X0-MS - System Control Descr.: The Air/Water Check is run at the end of every Auto-tune. If the masses 18 & 28 were not tuned, a message is now displayed in the Tune Report. If the Air/Water Check is run independent of the Auto-Tune and 18&28 are not tuned, a message is displayed indicating that an accurate Air/Water check relies on a current Auto-tune of masses 18 & 28.
Id: 6457	Title: Instrument status says 'Calibrating Methane' when it's actually Flushing. Area: 3X0-MS - System Control Descr.: When the system is switched from EI to CI, the correct status of Flushing is displayed.
Id: 6454	Title: EDR Calibration Problems Area: Quad - Status & Control Window – Auto Tune Descr.: Periodically, especially with new detectors, there are discontinuities in the EDR calibration due to the broad range of voltages included in the curve. The EDR calibration routine has been modified to eliminate this problem.
Id: 6443	Title: Inlet interlock cable disconnected should behave as open cap Area: 3X0-MS - System Control Descr.: When the Inlet interlock cable is disconnected, the filament, detector, and quad voltages are disabled as it does when the spray chamber is open.
Id: 6432	Title: Analyzer Connections test questionable Area: Quad - System Control Descr.: The “dirt test” from the Analyzer Connections test has been removed.
Id: 6431	Title: Uninitialized EEPROM on new power PCB should be initialized Area: Quad - System Control Descr.: When a new Power PCB installed on a Quad, the EEPROM will now be initialized automatically if a valid config.cub exists.
Id: 6407	Title: There is no 'EFC/EPC Check' Log Area: 3X0-MS - System Control Descr.: The new EFC/EPC Check log is a single file that is over-written each time the test runs. The user can now view or clear the log from the dialog.
Id: 6406	Title: Need to clarify Air/Water Check Criteria Area: Quad - Status & Control Window Descr.: The Air/Water Check is now run at the end of every Auto-Tune when operating in EI Mode. The Air/Water Check will no longer report the size of Mass 18 and Mass 28 in relation to Mass 69.
Id: 6404	Title: Q1ms and Q3ms switching isn't always immediately reflected in the status Area: Quad - Status & Control Window Descr.: After typing Q1ms in the command line and then switching to Q3ms, although scanning does change as it should to Q3ms, the status screen reflecting this isn't always updated until some other action is taken in the system. This has been corrected.

Id: 6403	Title: Manifold heater should be shut off if fuse F3 is blown Area: Quad - System Control Descr.: The Manifold Heater is now shut off if fuse F3 is blown.
Id: 6402	Title: Low end limiting of the RF is too restrictive Area: 3X0-MS - System Control Descr.: When scanning from mass 10, some systems will sometimes exhibit a ghost peak as a result of variances in Mass Calibration. This ghost peak as been eliminated.
Id: 6391	Title: Probe Status in Instrument Status screen gets truncated Area: 3X0-MS - System Control Descr.: If there are more than 2 numerical digits for the probe current/temperature, the text box in the instrument status screen gets cut off, so that the values are not visible. The text box has been updated so that all the digits are visible.
Id: 6388	Title: RunLog and Detector Overrides Area: Quad – System Control Descr.: The RunLog has been updated so that the Detector Voltage used in the method is documented correctly.
Id: 6387	Title: APCI Corona current resets on some Breakdown curves Area: 1200: System Control Descr.: This has been corrected so that current set in the method is used in the Breakdown.
Id: 6385	Title: Acquisition hangs on Waiting for Injection Area: Quad - Automation Descr.: When running a Sample List without an autosampler, after a number of injections, the acquisition/automation will get stuck on Waiting for Injection. This occurred when the Quad module was in the AutoStart window. This problem has been corrected.
Id: 6365	Title: If using all masses in Probe feedback mode, the incorrect mass range is scanned Area: 3X0-MS - Probe Descr.: If the "Intensity of ions scanned" Ion signal type is selected in Probe "feedback" mode (Changes temperature ramp to reach target ion signal strength), an incorrect mass range is evaluated. This has been corrected.
Id: 6364	Title: Exposure Probe maximum current is wrong Area: 3X0-MS - System Control - Automation Descr.: The Exposure Probe max current has been correctly changed to 1500mA.
Id: 6361	Title: Open Current Error if running Probe with automatic adjust to signal strength Area: 3X0-MS - Probe Descr.: If the Probe is running in "feedback" mode, an "Open Current Error" occurs shortly after initiating the program with a starting current of 10. This has been corrected.
Id: 6360	Title: Scan parameters changed during acquisition will not take effect if probe is running Area: 3X0-MS - Acquisition Descr.: When performing an acquisition with the probe running and the Scan Parameters (such as mass window) are changed, the message "Would you like to Install the new method into the scan?" is displayed. If you click on Apply, the changes are now applied correctly.
Id: 6344	Title: EDR Calibration Error Area: Quad – Auto Tune Descr.: The EDR calibration error currently tells the user that the calibration was aborted: "Curve - ion signal too large". A message box now tells the Operator to try the calibration again after 1 - 7 days if a new

	multiplier was just installed.
Id: 6334	Title: System Control Crash when syntax error occurs in Advanced Options PML command line Area: Quad - System Control Descr.: In the Advanced Options window of the Scan Table (in Manual Control), if a PML with incorrect syntax is entered, there is an error message displayed, but System Control hangs without allowing the error to be resolved. This has now been corrected.

CORRECTIONS IN MSWS 6.9 SP1

Id: 6322	Title: API voltages are set to minimum values on new install Area: 1200: System Control Descr.: The API voltages on a new install are now set as follows for POS: needle 5000, shield 600, capillary 100, and in NEG: needle -4500, shield -600, capillary -100.
Id: 6321	Title: Poor drying gas temperature performance when changing setpoints Area: 3X0-MS - System Control Descr.: In previous versions of the software, when the Drying Gas Temperature setpoint was changed, even if the new setpoint was close to the old one, the actual temperature dropped 5-10 degrees before recovering. Such perturbations have been reduced in this release.
Id: 6306	Title: EDR Calibration failure not identified Area: 3X0-MS - System Control Descr.: The EDR Calibration failure check was rendered ineffective in MSWS 6.9. As such, some failures of EDR Calibration would not be reported to the user. This EDR Calibration check has been restored in this release.
Id: 6310	Title: Retention Time Not Reproducible Area: Quad - Acquisition Descr.: In versions 6.8 and 6.9 of the software, the hardware Start In synchronization did not work, resulting in peak jitter of more than a second. The Start In synchronization has been fixed in the current release.
Id: 6311	Title: Baseline can sometimes drift toward zero Area: Quad - Status & Control Window - Acquisition Descr.: Two new PMLs have been included in the distribution: Baseline_lock increases the background by the specified percentage and locks it. Baseline_unlock goes back to the automatically calculated background level.
Id: 6293	Title: Printed Method doesn't contain PML information Area: Quad Method Descr.: In previous versions of the software, if the Quadrupole Method was printed from Method Builder, the PMLs specified for execution as part of each Method Segment are not listed. This has been corrected in the current release.
Id: 6298	Title: Pressing Enter after changing Polarity switches it back to original Area: Quad Method Descr.: In previous versions of the software, if the polarity of the ion is changed in the Scan Table and that is followed by pressing the Enter key, it switches back to the original value instead of preserving the change. This has been corrected in the current release.
Id: 6234	Title: Option to choose the current EDR Maximum detector value as a fixed setting Area: Quad Method Descr.: An additional detector voltage option has been added to the method in this release:

	EDR Maximum. When selected, it causes the system to use the last calculated EDR Maximum value, which is appropriate for use with low ion signal techniques, such as MS/MS. This option will automatically correct for the evolution of the multiplier performance over time. This option should not be used with Full Scan data as the detector will saturate.
Id: 6270	<p>Title: Duplicate Ions added to new methods during MS/MS breakdown and API Capillary</p> <p>Area: Quad: System Control</p> <p>Descr.: In previous versions of the software, if the MS/MS or API Capillary Breakdown is run with "appending of ions" enabled on a new method, two sets of ions result: One is correct and contains the capillary and collision energy information. The other has the same ions, but does not contain the capillary and collision information. This has been corrected in the latest release.</p>

Note: The following change to the Tune Report was implemented in MSWS 6.9 for Quadrupole MS systems:

If a problem is encountered with a mass that is specified to be included in the report but not tuned, the message "Reported only, not tuned" will appear in the report under that particular mass. If the mass is reported only and no problem is encountered, no message will appear.