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Varian MS Workstation Version 6.9.2 Release/Update Notes

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Overview

These Release Notes are organized into two broad categories:

- Items of Interest to All Users of the Varian MS Workstation Version 6.9.2
- Items of Interest to Users Upgrading from MS Workstation Version 6.9.1

All Varian MS Workstation operators should read the section “Items of Interest to All Users of the Varian MS Workstation Version 6.9.2.”

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 6.9.2

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 6.9.2 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 6.9.2 introduces a driver for the 216-LC nano-LC System (pump with integrated autosampler), and supports nanospray interfaces on the 500-MS and 310/320-MS models.

MSWS 6.9.2 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.

WINDOWS AUTOMATIC UPDATES AND COMMUNICATION FAILURES

Enabling Automatic Windows updates can lead to automated restarts that would interfere with automation runs. Under Automatic Updates in the Control Panel, We recommend you do not select the "Automatic (Recommended)" option, but instead use the next option "Download updates for me, but let me choose you 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

The MSWS software is installed with a set of two CDs, including a Setup disk and a Documentation disk.

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.

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.

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 6.9.2 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 6.9.2, serial numbers from pre-6.5 versions of the core MS Workstation software will not work with 6.9.2. You must purchase an upgrade to use the MSWS 6.9.2 software.

Update Ver 6.x to Ver 6.9.2 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 6.9.2, serial numbers from pre-6.5 versions of the core MS Workstation software will not work with 6.9.2. You must purchase an upgrade to use the MSWS 6.9.2 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 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.

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 6.9.2 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 6.9.2

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	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 whose data you may need to review.
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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 6.9.1

What's New in MSWS 6.9.2

The primary purpose of the MS Workstation 6.9.2 release is to provide drivers for the new 216-LC, and support a nano-spray source on the LC/MS models. These are used by the 920-MS, which uses a modified version of the MSWS.

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

MSWS 6.9.2 includes all of the changes and improvements implemented in HotFixes since MSWS 6.9.1.

Core Workstation Platform

NIST 08

The NIST 08 search program is used in MSWS 6.9.2

ENHANCEMENTS IN MSWS 6.9.2

Id: 6645	Title: Change extension of exported ion file from .mgf to .MGF Area: Exportions Descr.: The Export Ions Utility now exports ions to a *.mgf file instead of a *.MGF file so that all search vendors can read the exported file.
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Id: 6813	Title: Add command line option to convert CDF file to RUN Area: Advanced Applications Descr.: The CDFCONV application was extended so that it will accept a CDF file name on the command line and convert it into a RUN file.
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CORRECTIONS IN MSWS 6.9.2

Id: 6811	Title: Suspended recal list not updated correctly if single sample run before resuming Area: System Control - Automation Descr.: Upon resuming a Sample List after running a Single Sample Injection while the Sample List was suspended (e.g., handling a Priority Sample), data files were not properly added to the Recalc List specified in the Sample List. This problem was corrected in MSWS 6.9.2.
Id: 6795	Title: Exportlons Utility should remember its settings Area: System Control - Automation Descr.: The Exportlons program was modified to remember its settings, instead of reverting to default parameters on each session.
Id: 6846	Title: 450-GC: Output section should allow 25 rows Area: 450-GC Driver Descr.: The Method Editor was modified to allow 25 lines in the Output section of the 450-GC method – as available in the GC Local User Interface. Previously only 5 lines were available
Id: 6827	Title: Change EFC pressure limit to 150 psi Area: 450-GC Driver Descr.: The driver was corrected to allow EFC pressures up to 150 psi (previous limit was 100 psi)
Id: 6821	Title: Can't disable solvent plug in User Defined mode Area: 450-GC Driver Descr.: A checkbox was added to enable/disable the use of a solvent plug in the AutoSampler section of the GC method (under 'More User Defined Parameters' for 8400 and 8410)

200-MS & 2000 GC/MS Ion Trap Module Changes

ENHANCEMENTS IN MSWS 6.9.2

Id: 6758	Title: Modify CI Adjust operation Area: 200-MS and 2000-MS Descr.: The CI Adjust dialog has been modified to remove the progress bar, and to provide the operator with general guidelines about which ions should be displayed for different CI gases.
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CORRECTIONS IN MSWS 6.9.2

Id: 6414	Title: Change default Manifold temp from 80°C to 40°C Area: 2000 MS and 200-MS Driver Descr.: The code was changed to use 40°C as the default.
Id: 6851	Title: System Control is using too much CPU time during filament delay Area: 2000 MS and 200-MS Driver Descr.: The code was changed to avoid monopolizing the CPU during filament delay.

Id: 6669	Title: 200-MS data files cannot be read by AMDIS Area: 200-MS Descr.: The latest version of AMDIS (included with NIST08) can read 200-MS data files
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4000 GC/MS Ion Trap Module Changes

GENERAL INFORMATION

Hybrid method for mass check

A method entitled "hybrid_MassCheck.mth" check has been added to the 4000Service folder in the VarianWS directory. This provides a check of the mass calibration in Manual Control for the hybrid mode of operation. This method is needed to compensate for the removal of "Mass Check" in hybrid mode in the "Checks & Adjustments" tab.

CI Adjust Dialog

The CI adjust dialog has been changed. The progress bar has been removed. The user is given guidelines for optimization based on the CI gas. In external mode, the ion gauge pressure is displayed. In the Run Log/Module Attributes, the Result will be "Complete" instead of Low, High, or Ok.

500 LC/MS Ion Trap Module Changes

Initial Conditions in Manual Control

When a temperature ramp (APCI/ESI/nESI) or Emitter voltage ramp (nESI) is enabled in the active method while in manual control, the temperatures and emitter voltage will be set to the initial ramp conditions.

In previous versions of MSWS, the temperature at the end of the ramp would be set in manual control for ESI and APCI.

ENHANCEMENTS IN MSWS 6.9.2

Id: 6733	Title: AutoLink command for .MGF file generation Area: LC/MS Descr.: The ExportIons program can now be used to automatically create a *.mgf file. This *.mgf file can then be exported into mascot for database searching. The AutoLink command works through a Sample List or Recalc List. The AutoLink command line is "exportions -rai".
Id: 6643	Title: Make API temp and voltage ramps go to initial conditions in Manual Control Area: 500-MS driver Descr.: (As discussed above under <i>Initial Conditions in Manual Control</i>)
Id: 6559	Title: Remove Autotune and Checks and Adjustments tab with APCI Area: 500-MS driver Descr.: For APCI configurations, there is no longer an Autotune tab or Checks and Adjustments tab.
Id: 6243	Title: Eliminate need to acknowledge message boxes for housing connect/disconnect Area: 500-MS driver Descr.: The message box that is displayed after disconnection/reconnection of the housing will now disappear after 3 seconds. The user no longer has to click ok.

Id: 6154	Title: Change default APCI temp from 50°C to 65°C Area: 500-MS driver Descr.: The default housing temperature for APCI has been change from 50°C to 65°C.
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CORRECTIONS IN MSWS 6.9.2

Id: 6744	Title: Syringe pump flow resolution Area: 500-MS Control Method Descr.: The syringe pump flow display has been changed to show two decimal places
Id: 6723	Title: Editing 2 methods simultaneously can cause crash Area: 500-MS Method Editor Descr.: It is now possible to edit two or more methods with 500-MS sections

MS Data Handling Changes

CORRECTIONS IN MSWS 6.9.2

Id: 6809	Title: Method gets "modified" during processing of analysis files Area: MS Data Review – Quan, Review Results Descr.: Corrected a problem in which method file time stamps were updated during the processing of analysis files.
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Quadrupole MS Module Changes (1200/1200L/300-MS/310-MS/320-MS)

GENERAL INFORMATION

Acquisition Method Changes

The Acquisition Method was extended to support 60 segments (previously supported only 40 segments).

CORRECTIONS IN MSWS 6.9.2

Id: 6782	Title: Changing Vaporizer Pressure in System control doesn't take effect Area: 3X0-MS - System Control Descr.: Changing the Vaporizer Gas Pressure from within the Instrument Status Window didn't work in a previous version. This has been corrected in the current release.
Id: 6751	Title: Indefinite CI Flushing. Area: 3X0-MS - System Control Descr.: An error that resulted in an indefinite CI flush when switching from EI mode before CI gas calibration has been corrected.
Id: 6750	Title: Hardware Diagnostics can fail if begun in negative mode Area: 3X0-MS - System Control Descr.: The scan conditions have been automatically set to eliminate false failures of the shield voltage.
Id: 6743	Title: Syringe pump flow resolution Area: 3X0-MS - System Control Descr.: The syringe flow rate display has been changed to show 2 decimal places.

Id: 6742	<p>Title: 3XX Single Quad CID Pressure</p> <p>Area: 3X0-MS - System Control</p> <p>Descr.: The software no longer reports an error about CID pressure being present in the single quad system.</p>
Id: 6654	<p>Title: CID Ready Status</p> <p>Area: 3X0-MS - System Control</p> <p>Descr.: When the user turns on the CID gas, the pressure that is observed in the Instrument Parameters view may not be at the setpoint, but the instrument says it is ready. The pressure reading that is shown in the software is being read from a Convectron Gauge.</p> <p>The Convectron Gauge is not used to determine the ready status of the CID gas pressure (because it is slow and only effective in steady-state conditions). An internal electronic pressure controller is used to determine when the CID pressure is ready.</p>
Id: 6731	<p>Title: Start-In Hardware Signal for Quad not working</p> <p>Area: 3X0-MS - System Control</p> <p>Descr.: In MSWS 6.9.1, the start-in signal for the Quad did not work correctly. This was fixed in the current release.</p>
Id: 6374	<p>Title: CID not turned back on after startup of System Control if active in method</p> <p>Area: 3X0-MS - System Control</p> <p>Descr.: System Control will turn on the CID gas if the last active method before system shutdown specified CID gas on. In previous versions, the CID gas would be turned only after method activation through sample injection or through reactivate method.</p>