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Varian MS Workstation Version 6.8 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 6.8
- Items of Interest to Users Upgrading from MS Workstation Version 6.6

All Varian MS Workstation operators should read the section "Items of Interest to All Users of the Varian MS Workstation Version 6.8."

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 6.8

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.
- 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

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 lowusage 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.

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 defragmentation and deleting old .TMP files in your tmp or temp directories 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 privilege 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 6.8 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 6.8, serial numbers from pre-6.5 versions of the core MS Workstation software will not work with 6.8. You must purchase an upgrade to use the MSWS 6.5 (or later) software.

Update Ver 6.x to Ver 6.8 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 6.8, serial numbers from pre-6.5 versions of the core MS Workstation software will not work with 6.8. 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 1200 MS Module Driver has been renamed "Quad Mass Spec" as it now supports multiple models of quadrupole MS modules (1200, 1200L, 310-MS, and 320-MS). As such, that is how it will appear in all areas of the software.

At the end of the installation, turn off the computer and install any interface cards required for your hardware (Kodiak 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 6.8 software. Optional software such as ToxProPlus 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

MULTIPLE USERS OF 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 therfore 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 accesible by all Wokstation 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 in use in two applications simultaneously. In particular, methods used for automated acquisition and data handling in System Control should not also be opened with Method Builder simultaneously.

A method should not be modified in another application while the results that were generated by it are displayed in the Results View in MS Data Review. Since the modified method may no longer be consistent with the results, a message will be displayed stating that the method has changed and that the Results View must be updated. The Results View display will be cleared when the dialog is OK'd. You should go to the Process View to reprocess the file with the newly-modified method, and then return to the Results View to view the updated results.

If the results in a Recalc List are being displayed in the Results View at the same time that they are being generated in System Control, the "Method has changed..." message will be displayed each time that processing on a file is completed and the Results View display will be cleared when the dialog is closed. In most cases, the simplest solution is to go to the Results View to view the results after all processing has been completed. If you must view the results while they are being generated, first make a copy of the method, reprocess the recalc list in the Process View with the copy, and then go to the Results View to view the results. The "Method has changed..." message won't be displayed because a "different" method (that is, a copy) is being used.

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 330 PDA

If both the Saturn 2000 and PolyView 2000 are selected for installation, then the Saturn 2000 will be installed with data handling capability only. As the Saturn 2000 and 330 PDA (installed with PolyView 2000) 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.

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.

Items of Interest to Users Upgrading from MS Workstation 6.6

What's New

The primary purpose of the MS Workstation 6.8 release is to provide an upgraded Quadrupole Module Driver that includes new features for 1200 users and support for the new 3X0-MS Quadrupole Module. Further improvements and corrections to the MS Data Handling features introduced in MS Workstation 6.5 have been included as well.

New products released at or about the same time as 6.8 include the Quick Access software, Mass ID[™] Deconvolution Software for multiply charged ion spectra, and 212-LC Pump System Driver. These are described separately.

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

IMPROVEMENTS

Acquisition Method Changes - General

The Acquisition Method has been substantially changed from previous versions.

In order to better support Model and Ionization-specific parameter validation, the MS Model Number and Ionization Type have been added to the method.

A number of previously unavailable parameters may now be controlled or "overridden" in the method. These are accessed by clicking on the "Advanced

Options" button in the lower left of the Ion Dialog. Doing so brings up a tabbed dialog with options appropriate to the Model and Ionization Type specified.

A number of the Source Parameters and other hardware elements may now be controlled via the method from the Advanced Options Dialog.

A new Collect Data checkbox is available that can be used to prevent data collection during certain method segments.

A new Syringe On checkbox is available (on 320-MS only and if enabled) that can be used to turn on/off the Syringe Pump on a method segment basis.

In previous versions of the Method, there were two separate Scan Method and Acquisition Method sections. In this release, these have been combined into a single method section.

Acquisition Method – GC Advanced Options

When configured for GC ionization, the Advanced Options dialog contains the tabs and parameters listed below:

Overrides
Detector Voltage
Source Temperature
CID Gas Pressure*
("Ready

("Ready" Criterion Only on 1200/1200L)

Acquisition Method – LC Advanced Options

When configured for LC ionization, the Advanced Options dialog contains the tabs and parameters listed below:

• Overrides

Detector Voltage Corona Current (Positive/Negative) – APCI Only Needle Voltage (Positive/Negative) – ESI Only Spray Shield (Positive/Negative) Spray Chamber Temperature Drying Gas Temperature Vaporizer Gas Temperature – APCI Only CID Gas Pressure* ("Ready" Criterion Only on 1200L) Nebulizing Gas Pressure* ("Ready" Criterion Only on 1200L) Drying Gas Pressure* ("Ready" Criterion Only on 1200L) Vaporizer Gas Pressure* ("Ready" Criterion Only on 1200L)

• Drying Gas

Temperature Program

• Vaporizer Gas – APCI Only

Temperature Program

• Valve – 1200L Only

Use of the Six-Port Valve (Manual, Diverter, Injector) Load Position required for ready state

• Valve and Syringe Pump – 320-MS Only

Use of the Six-Port Valve (Manual, Diverter, Injector)

Load Position required for ready state

Syringe Pump Flow Rate

Turn off Syringe Pump at end of Method

Acquisition Method – General Advanced Options

All Models/Ionization Types include the following tabs and parameters on the Advanced Options dialog:

• User Analogs In/Out

Analog Output #1 (TIC and TIC x N)

Analog Output #2 (TIC and TIC x N)

Collect User Traces

- User Input 1
- User Input 2
- User Input 3
- Readback
- PML
- PMLs

Per-Method Segment PMLs

Post-Run PML

Acquisition Method – Mass List Spreadsheet

The previous pseudo Mass List table has been replaced with an actual spreadsheet that supports the usual spreadsheet functions. Add – Add a new row to the end of the table.

Insert – Insert a new row before the current row.

Delete - Delete the currently-selected row.

Clear All – Clear the whole mass list table.

Cut – Make a clipboard copy and delete the current row.

Copy – Make a clipboard copy of the current row.

Paste – Paste the clipboard data into the currently-selected row.

Fill Down – Fill down the selected column(s) in the selected rows.

<u>Caveat</u>: In MS Workstation 6.8, the keyboard accelerator keys Ctrl+C and Ctrl+V should not be used in place of the Copy and Paste functions in the Mass List Spreadsheet, nor when copying or pasting between Microsoft Excel and the Mass List Spreadsheet.

Acquisition Method – Requested Dwell Time

The user may now specify a requested Dwell Time for each separate transition in the Mass List table. However, the actual dwell time used may vary from the requested dwell time, depending upon scanning conditions. This is most pronounced when scanning multiple mass ranges in a single method segment; all such scanning must occur at the same scan speed and the system will make the required adjustments automatically when running in System Control.

<u>Caveat</u>: For best results, any method created with a previous MS Workstation release should be opened with Method Builder, the system-calculated requested dwell times in each segment verified/adjusted by the user, and the updated method re-written to disk prior to running an acquisition.

Acquisition Method – Capillary CID

If an LC/MS is configured with a Quadrupole Ion Guide, the user may specify a different Capillary CID for each transition. Otherwise, only a single Capillary CID value for the Method Segment is allowed

Status View Window

The Status View Window has been updated with new status fields, buttons, and icons to support the status and control of the new features in the 3X0-MS. Which elements are present in the display depends upon the Model and Ionization Mode currently in use. In addition, the Quadrupole graphic itself has been updated to more closely reflect the actual instrument.

Probe Control

Probe control has been eliminated in this release.

Capillary Breakdown Tool

The existing MSMS Breakdown Tool has been expanded to support a similar function using the Capillary on LC/MS systems.

For both functions, the N highest ions may now be added to the specified Quadrupole MS Workstation Method as opposed to the now-obsolete "Ion File." At present, these methods must reside in the \VarianWS\Methods subdirectory.

Repartitioning of Diagnostics/Troubleshooting/Setup Functions

The Diagnostics/Troubleshooting/Setup features previously located on the File... menu have been re-organized and moved to new options (Troubleshooting, Inst Setup/Others) on the Tools... menu.

New Ready Conditions and Warnings

The desired API Pressures may now be specified in the Method and the system will ensure that these specifications are satisfied before the module becomes Ready to acquire data.

View Reports

The Reports menu provides a way to create printouts of the 5 User Defined Views.

Revised Tune To Target Ratios Function

Ion Ratios may now be tuned from live Calibration Gas spectra in addition to previously acquired data files.

When you click on "Tune to Ratios" you get a much simpler, two choice menu:

- 1- "Tune Calibration Gas Ratios Directly". (This part is new.)
- 2- "Use a previously acquired data file (DFTPP, etc.)". This part existed since 6.4.2 but has now been revised.

You also get to choose what compound you want to tune on and what are the ratio ranges. There are predefined files with some common compounds (BFB 524, DFTPP 525, FC-43) and the user can also make and save its own.

The new part "tune on calgas" is the preferred one and it should bring the operation closer to competitive instruments. When you chose this part, you are first advised that you need to have no air leaks and that you need to autotune before you run this. Once you say "OK", it runs, measures current ratios, calculates adjustments, then tunes Lens 3 and eliminates some masses in order to adjust ratios. During the tune it plots the tuning curves and at the end it makes a report in pict, pops up a window with final ratios, and asks you if you want to save this tune. The whole process is relatively short, including the wait for the calgas to stabilize if it was not already on.

If the adjustments require reducing more than 40% of intensity at any ion, then a dialog appears asking if you really want to do this (or if you should check for leaks, autotune or clean the source). You have the option of going on.

Reconfigured Traffic Light ("Collect Data") Dialog

A number of the parameters previously specified from the Traffic Light Dialog (e.g., End Time) have been moved to the Method and have, therefore, been removed from the former. The Scan Method now refers to a Quadrupole MS Workstation Method as opposed to a now-obsolete "Ion File." At present, these methods must reside in the \VarianWS\Methods subdirectory.

Eliminated Superfluous Options

A number of redundant and superfluous options on the Chromatogram, Profile, Centroid and Spectra Windows were removed. These functions should now be performed from the MS Data Review application.

The Library Window and Mass Map windows were eliminated. The functions should now be performed from the MS Data Review application.

New Air/Water Check Function

There is a new Air and Water Report function available from the Tools/Trouble Shooting Dialog.

Simplified Sync Signal Dialog

The default Sync Signal Dialog is now simpler. The Advanced button must be pressed to display the full wiring diagram.

Run Log Additions/Reformatting

There has been some reformatting and repartitioning of the elements within the Run Log.

Tune without Cal Gas On

Auto Tuning may now be completed without having the Cal Gas on. There is a new checkbox on the Auto Tune Dialog to enable/disable Cal Gas.

Tune Report Format Changes

The format of the Tune Report has changed somewhat. The columns displayed have changed and criteria and warnings for Mass Accuracy and Resolution have been added.

User Selection of Pressure Units

In previous versions of the software, the User Selection of Pressure Units feature was not completed. Not all displays followed the user-specified units. In this release, all pressure displays follow the user-specified units.

Various Improvements to Diagnostic Functions

A number of improvements have been made to the various Diagnostic Functions within the module to make them more reliable and to provide better diagnosis of problems.

KNOWN ISSUES

The following are issues with which the user should be familiar and take precautions to avoid:

ld: 5652	Title:	Running more than one automated function at the same time can cause one or both to fail.
	Component:	Quad
	Area:	ModWin - General
	Description:	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.
ld: 5899	Title:	Manually changing operating conditions while automated functions are running can cause them to fail.
	Component:	Quad
	Area:	ModWin - General
	Description:	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.
ld: 5782	Title:	Keyboard accelerators for Copy/Paste don't work properly in Mass List Spreadsheet.
0.01	Component:	Quad
	Area:	ModWin - General
	Description:	The keyboard accelerator keys Ctrl+C and Ctrl+V should not be used in place of the Copy and Paste functions in the Mass List Spreadsheet, nor when copying or pasting between Microsoft Excel and the Mass List Spreadsheet as the data will not be properly transferred.

2000 GC/MS Ion Trap Module Changes

IMPROVEMENTS

ld:	Title:	MRM and MSMS combined
3999	Component:	2000
	Area:	DAMeth - MSMS

	Description:	When using MRM the user is just doing two or more MSMS experiments; or to take this further, MSMS is the superset of both SRM and MRM and the two modes are defined by the number of trasitions specified. It might be easier for the user if the 2000 software only had a single MSMS function that changed from SRM to MRM if a second line was added to the method.
ld: 5080	Title: Component: Area: Description:	Purge B files for Service directory 2000 Installation/Configuration The PurgeB methods for the 2100 and for the 2200 have been updated. An example data file is also included.

CORRECTIONS

ld:	Title:	Handle Leak in System Control due to 2000 Module Login
4817	Component:	2000
	Area:	ModWin - General
	Description:	When the 2000 module attempts to login in, but the MS is not connected to the system, a handle is leaked. This occurs with each attempt and may eventually reduce the availability of Windows resources.
ld:	Title:	Invalid Flow Sampling Period Allowed
2592	Component:	2000
	Area:	DAMeth - General
	Description:	The Saturn 2000 Special Application Dialog allows Flow Sampling Periods outside of the documented range of -10.0 to 0.00 minutes. When the flow sampling period exceeds 10 minutes, the calculated result is in error.
ld:	Title:	Customize dialog not updated for resonant/non-resonant change
5307	Component:	2000
	Area:	DAMeth - MSMS
	Description:	Create a new 2000 MS method. Set a segments ionization mode to EI Auto and its ion preparation to MS/MS. Go to the MS/MS tab and click the waveform type to change it from resonant to non-resonant. Click to turn it back to resonant. Click the customize button. It shows the non-resonant MRM dialog. After that, clicks to the Resonant button are ignored, unless segments are changed.

4000 GC/MS Ion Trap Module Changes

IMPROVEMENTS

Auto Tune Summary Report

In the Auto tune mode It is now possible to view a report of the last auto tune results directly in the module window. In the drop down list box, select "Summary Report." If the tunes have been run on the instrument, a report of the results will be displayed. Clicking the "Print" button will print the report.

ld:	Title:	Replacement 4000 PurgeB method files
5081	Component:	4000
	Area:	Installation/Configuration
	Description:	The External PurgeB.mth and the Internal PurgeB.mth methods have been updated; some minor changes to the method notes and compound table

		entries were made.
ld:	Title:	CI emission current should be restricted
4572	Component:	4000
	Area:	DAMeth - CI
	Description:	Currently, the emission current in internal CI mode can be set to 100 uA. We'd like to restrict the emission current range to be 5-50 uA instead of 5- 100 uA. Internal EI and all external modes are unaffected.
		A separate SCR (4571) has been written to change system verification to test to this new limit.
ld:	Title:	Electron Lens autotune can fail to find correct tuning
5239	Component:	4000
	Area:	ModWin - Auto Tune
	Description:	The attached file shows a case in which this problem occurs. The relevant part of the file is below.
		Apr 27 16:01:07: Slope Diff: 685.00 (uA/sec) RMS: 24 (0.1 uA)
		Apr 27 16:01:07: EI Electron/Repeller Lens Tuning Failed
ld:	Title:	Change maximum trap temperature limit
5360	Component:	4000
	Area:	ModWin - Temperatures
	Description:	The 4000 MS Performance CAT has determined that the electrodes need to operate at 240 degrees to properly handle the most difficult pesticides from a tailing standpoint. Experiments have shown that in order to achieve that temperature the trap ovens must run at 265 degrees. The current software limits the maximum oven temperature setpoint to 250 degrees. In order to be able to achieve the desired temperature this limit should be changed to 270 degrees anywhere that there is a trap temperature limit in the software. The upper limit trap temperature is 270 for systems with Power Board version greater than zero.

CORRECTIONS

ld: 3179	Title:	Emission Current not reported correctly in Run file's MS Acquire segment Log
	Component:	4000
	Area:	MSDataRev - General
	Description:	In External Mode the emission current is not reported correctly.
ld:	Title:	User always receives an error on system startup
4472	Component:	4000
	Area:	ModWin - Shutdown
	Description:	The temperatures are set to the setpoints after the vacuum is ready and immediately after they are set quick verify is run. The heated zones will not be at the setpoint yet and the user will always get error messages on startup.
ld:	Title:	Board versions aren't reported correctly in Module Attributes
3727	Component:	4000
	Area:	System Control - General
	Description:	The list of module attributes reported has an entry for "Controller Board Version" and another entry for "Other Board Versions" which are reported incorrectly.
ld:	Title:	Air/Water Check needs to be Improved with New Electrodes
4683	Component:	4000
	Area:	System Control - General

	Description:	INTERNAL MODE- With the new electrodes the fixed ion time of 300 uSec
		is too small for some systems and shows no spectra.
		EXTERNAL MODE- the signal is too low giving false negative for 19/18 ratio.
ld:	Title:	AMD to MSMS gives two entries
4520	Component:	4000
	Area:	DAMeth - MSMS
	Description:	When switching from AMD to MSMS and you have selected a line, the MSMS parameters show two, identical, lines. In this situation there should only be 1 line transfered.
ld:	Title:	Switching modes has wrong source temp defaults
4854	Component:	4000
	Area:	ModWin - Temperatures
	Description:	When swaping the 4000 GC/MS from internal to external the default source temp is set to 0C (or blank).
ld:	Title:	4000 file crashes MS Standard Reports
4973	Component:	4000
	Area:	MS Report Application
	Description:	MS Standard reports crashes when some files are selected. When the file is
		loaded into MSDR and the log info is accessed, MSDR either displays
		"Could not format run log for the module at address" or hangs MSDR with a (Not Responding indicator).
	Title:	Incorrect values are automatically computed for the 4000 in AMD,
ld: 4983		MS/MS, and MSn
4905	Component:	4000
	Area:	DAMeth - General
	Description:	The AMD, MS/MS, and MSn parameters should not be automatically computed.
ld:	Title:	4000 Target TIC still editable when in fixed ionization mode
5248	Component:	4000
	Area:	DAMeth - General
	Description:	For the 4000MS, when switching from AGC to fixed ionization mode, the Target TIC name becomes grayed out but the counts field remains editable. These edits do not actually do anything, but the field should be grayed out also to remain consistent.
ld:	Title:	Integrator zero report discrepancy
5238	Component:	4000
	Area:	ModWin - Auto Tune
	Description:	The integrator zero autotune displays says that the acceptable limits for the
		average intensity is between 0.3 and 0.5. Occasionally the autotune will
		pass despite the average intensity being reported as less than 0.3 (I haven't seen this happen for the case that the average is more than 0.5).
ld:	Title:	Max. ion. time is not updated when switching form El to Cl
5140	Component:	4000
	Area:	DAMeth - El
	Description:	Go to create a new 4000 method. Select EI as ionization mode. Into the
		ionization control, click "customize" and you can see 25,000 usec as max.
		ionization time. OK. Now, change ionization mode to CI. Now you can see
		2,500 usec as max ionization time. OK. Now, come back to EI, maximun
		ionization time remain at 2,500 usec as CI. WRONG. This bug can create so many problems when customers are creating 4000 methods. Because max.
		ionization time is hidden(need to click "customize"), you never directly see
	•	

the max time that system is using. Last week, injecting pesticides samples from CNTA to check sensitivity in EI, I observed ten times less sensitivity than expected. I repeat several injections: same problem. Then, checking the method I saw that max. ionization time was 2,500 usec, because this
bug.

500 LC/MS Ion Trap Module Changes

IMPROVEMENTS

Auto Tune Summary Report

In the Auto tune mode It is now possible to view a report of the last auto tune results directly in the module window. In the drop down list box, select "Summary Report." If the tunes have been run on the instrument, a report of the results will be displayed. Clicking the "Print" button will print the report.

ld:	Title:	No method information saved in data files recorded in Manual Control
4144	Component:	500-MS
	Area:	MSDataRev - General
	Description:	No method/module atributes information is available for data files recorded in Manual Control, when right- clicking on the file name (data file pane in MSDR) and selecting Information/Show Logs
ld:	Title:	Need to Proivide for Reset of the Turbo pump lifetime counter
4561	Component:	500-MS
	Area:	ModWin - Diagnostics
	Description:	There needs to be a means to reset the turbo pump lifetime counter. Including a "This should only be done when installing a new turbo pump, are you sure you want to do this" message would probably be a good idea. If the pump controller is replaced, the counter will automatically be reset.
ld:	Title:	Add linear step to optimization plot
4378	Component:	500-MS
	Area:	ModWin - Manual Control
	Description:	Add a check box to the optimization plot dialog to allow for a linear step through the range.
ld:	Title:	Have quick verify check polarity switching
4778	Component:	500-MS
	Area:	ModWin - Diagnostics
	Description:	Quick Verify should do a polarity switching check to determine if the dynode voltage is set to 'normal' or to a fixed polarity in the advanced Module Attributes.
ld:	Title:	Make the Intensity Normalization Radio Buttons Less Accessible
4828	Component:	500-MS
	Area:	ModWin - Manual Control
	Description:	The ability to disable normalization of the intensities by ion time is too obvious and leads to confusion. Hide these controls behind a button.
ld:	Title:	Clicking the button would bring up a dialog with the radio buttons.
ia: 4829		Make Docking Window Visibility Easier 500-MS
7023	Component: Area:	ModWin - Manual Control
	Description:	When a user has closed a docking window, it takes 3 clicks to bring it back.
		One to bring up the dialog, one to select the window, and another to click

		OK. This could be simplified by putting the check boxes and a button for the default configuration right on the segment control bar.
ld:	Title:	Check invalid parameter on boot
4274	Component:	500-MS
	Area:	ModWin - General
	Description:	Dave DeFord is requesting this SCR. The request is to check the software system status word on boot to see if there are any invalid parameters per EFC/EPC module. Report this back so it is more obvious that there is something wrong with the EPROM.
ld: 5228	Title:	Remove the autotune for the ion guide RF amplitude and set the value to 230Volts
	Component:	500-MS
	Area:	ModWin - Auto Tune
	Description:	One of the more common failures when autotuning is the tuning of the ion guide RF amplitude. The routine can fail for a variety of reasons, but always tells the user to clean the ion optics when it fails, which may or may not solve the problem. After surveying the values set on all instruments to date (see attached file), it appears that we would be better served by just setting the ion guide RF amplitude to 230V. The verification routine should still look at both ends of the spectrum to make sure they are visible (i.e. m/z 74 and m/z 1922.)

CORRECTIONS

المار	Titles	Qualemental Waveform Turing machines on the 500 MQ
ld:	Title:	Suplemental Waveform Tuning problems on the 500-MS
4927	Component:	500-MS
	Area:	ModWin - Auto Tune
	Description:	Auto Tune is run and passed with no errors. When new method is activated an error message is generated saying: "Some Auto Tunes not up-to-date" and acquisition is not allowed.
ld:	Title:	Turn off multiplier when the spray chamber is opened
4932	Component:	500-MS
	Area:	System Control - General
	Description:	All of the voltages and gas flows are turned off when the spray chamber is opened, with the exception of the electron multiplier. To prevent potential damage to the multiplier during a capillary flush, it must be turned off as well.
ld:	Title:	Don't delete customer methods when installing software
4933	Component:	500-MS
	Area:	Installation/Configuration
	Description:	Currently, all customer methods contained within the 500-MS Methods directory are deleted without warning upon software installation. The standard methods should be restored and any changes to them discarded, but there is no need to totally clean out the directory.
ld: 4687	Title:	An icon, M, for the chromatogram display works differently in manual control and in acquisition
	Component:	500-MS
	Area:	ModWin - Manual Control
	Description:	The icon in Manual control in the Chromatogram display, when clicked in manual control pauses the update of the chromatogram. This icon should be removed and the updating of the chromatogram should be paused by the user zooming in on the area of interest.

ld:	Title:	Ion source and optics values should be displayed.
4709	Component:	500-MS
	Area:	ModWin - Diagnostics
	Description:	Ion Source and Optics Monitoring values should be scanned and displayed along with their setpoint values. This needs to be implemented.
ld:	Title:	500MS: Grayed-out AMD dialog
4774	Component:	500-MS
	Area:	ModWin - General
	Description:	After editing different segments and switching between the Method tab and the Active Segment tab, the AMD Parameters dialog appeared grayed-out with only one cell highlighted (selected but with no text).
ld: 4877	Title:	Foreline Pump Temperature Reading should be removed from diagnostic page
	Component:	500-MS
	Area:	ModWin - Diagnostics
	Description:	The foreline pumps no longer report the temperature, so the field should be removed from diagnostics.
ld:	Title:	Optimization fitting curve appearance during the optimization process
4882	Component:	500-MS
	Area:	ModWin - Manual Control
	Description:	At some instant at the beginning of the optimization process, while the points
		are added in, the fitting curve has a strange shape, intersecting the origin a couple of time.
ld:	Title:	Integrator Zero bad setting crashes 500MS
5018	Component:	500-MS
	Area:	ModWin - Auto Tune
	Description:	An instrument failed auto tune leading to a crash. On restart, the system fails
		again due to a bad value for integrator zero in the module attributes inside the startup.ins file.
ld:	Title:	Editing Low/High Offset parameters for all MS/MS type methods
4174	Component:	500-MS
	Area:	DAMeth - MSMS
	Description:	Low/High Offset parameters can be edited when Customize tab is clicked in the AMD/(MS/MS)/MS^n Parameters sections. For the Low Offset, values
		higher than 2 or lower than -2 cannot be entered and no message with admissible range is displayed. This message is however displayed when
		values in the range (0.8 - 1.0) or (-1.00.8) are entered. For the High
		Offset, no message with the admissible range is displayed for any value
		entered outside this range. The admissible range of values should be displayed for both parameters when values outside this range are entered.
ld:	Title:	500-MS quick verify in constant cycle in diagnostics
4969	Component:	500-MS
	Area:	ModWin - Diagnostics
	Description:	Start the Quick Verify daiagnostic test in the 500-MS diagnostics tab when
		the test is completed, it immediately starts again, and again, and again. Hitting the 'Stop Diagnostic' button does not stop this endless cycle. No
		other tabs can be accessed and stopping System Control from the task
		manager is the only option.
ld:	Title:	AMD and 500-MS
4670	Component:	500-MS
	Area:	DAMeth - AMD
	Description:	When you switch to the AMD tab, the default mass of 131 appears for rows

		4. C. If you show the many the Fundle Control And Physics and
		1-6. If you change the mass, the Excitation Amplitude does not automatically update in rows 2-6, while all the other parameters are updated with the change of mass.
		The Excitation Amplitude can be changed manually by the user. For AMD, it would be useful if the Excitation Amplitude was stepped in a certain increment (0.1 for example) around the "optimum value" created in row 1, and this was automatically entered into the Excitation Amplitude column.
ld:	Title:	Record Data operator field has extra characters
4476	Component:	500-MS
	Area:	ModWin - Manual Control
	Description:	If there is a name in the Operator field of the Instrument parameters and a Record Data session is run, in MSDR the log of this data file will show the Operator name in the field, but it will be followed by several block graphic characters. If you view a Standard MS Report of this data file, these characters are crosses. This doesn't happen during a regular acquisition.
ld:	Title:	New points not added to zoomed optimization plot
4356	Component:	500-MS
	Area:	ModWin - Manual Control
	Description:	When the user is zoomed in on a subset of the tune plots, new points are not added to the zoomed in section, even if they would have been displayed in the zoomed in section had they existed at the time of zooming. New points that are within the zoomed in area should be displayed when they are sent to the control. New points that are outside of the zoomed area should not cause the display to be changed, until the user selects full scan again or a zoomed in range in wich the points would be visible.
ld:	Title:	Method Builder crashes after right-click help for Defaults
5151	Component:	500-MS
	Area:	DAMeth - General
	Description:	Method Buider crashes after displaying help for the Defaults button by right- clicking on it. See the attached gpf file.
ld: 5152	Title:	Method Builder crashes when Restore is used after adding time segments
	Component:	500-MS
	Area:	DAMeth - General
	Description:	Method Builder crashes when the Restore button is pressed after adding time segments.
ld:	Title:	Default value for RF Loading
5153	Component:	500-MS
	Area:	DAMeth - General
	Description:	Deafault values exist for all scan parameters except the RF Loading. We should have the 100% value for the RF Loading default.
ld: 5154	Title:	Method Builder crashes when adding time segments after Divert/Load are selected
	Component:	500-MS
	Area:	DAMeth - General
	Description:	Method Builder crashes in the following circumstances: Select Diverter or Injector in Special Applications dialog and then check the Divert/Load checkbox and save the method. Adding time segments after this causes the crash. I think the application cannot decide consistently whether to keep the Divert/Load checkbox checked or not for the newly added segments.
ld: 5164	Title:	Some tabs in Manual Control can not be accessed after Recording Data

	Component:	500-MS
	Area:	ModWin - Manual Control
	Description:	After recording data in Manual Control the following tabs can not be accessed: Checks & Adjustments, Module Attributes and Optimization Plots. After you go under any other tab than Manual Control (Acquisition, Diagnostics,) and come back, these tabs can be accessed.
ld: 5181	Title:	Syringe on/off & 6 Port valve state at segment level in Standard Reports
	Component:	500-MS
	Area:	MS Report Application
	Description:	The configuration of the 6 Port Valve (Divertor/Injector/Manual) and use of Syringe Pump are documented in Standard Reprts (they are settings at Method level). At Segment level however, the state of the 6 port valve (Load- On/Off or Divert- On/Off) and Syringe On/Off are not documented in Standard Reports.
ld:	Title:	Failed to Load the Method Configuration Data
4227	Component:	500-MS
	Area:	System Control - General
	Description:	After a new installation or an installation where the startup.ins file has been deleted, the first time you run system control (going into the manual control screen) the module window displays the message, "Failed to Load the Method Configuration Data." The famous "Reset" button is also displayed. You must close the system and come back in to be able to run the module window.
ld:	Title:	System Control crashes during Auto tune while MSDR open
4963	Component:	500-MS
	Area:	ModWin - Auto Tune
	Description:	Auto tune was run while MSDR was kept open. System Control crashed at some point.

MS Data Handling Changes

IMPROVEMENTS

Enhancements to Updating Directory Tree Display in Data Files Pane

Several changes have been made to improve updating the display of the directory tree in the Plots View Data Files pane:

- An "Automatic Updates" tab has been added to the Plots View Preferences dialog to let users specify whether to do automatic updating, and how often. Previously, automatic updating always happened, and was done every 10 seconds. Now it is disabled by default. When enabled, the default update frequency has been changed to every 2 minutes.
- If a directory that is expanded in the Data Files pane contains more than 1,000 data files and recalc files, a message will be displayed that lists the number of files in the directory and suggests that the number be decreased to improve performance. This message will only be displayed once until MS Data Review is closed and then started again. The message can be disabled completely on the Automatic Updates tab in the Plots View Preferences dialog.
- An "Update Tree" button has been added below the Data files pane to allow users to update the display at any time.

• Updating now happens significantly faster when it does occur, especially when the expanded directories contain many files or are on a network drive, and the directory tree display also is initialized faster during application start-up.

Able To Adjust Integer-Mass Rounding for Library Searching

When fractional masses are rounded to integers (primarily for library searching), the mass peak window that's used is - 0.5 to + 0.499999 centered around the integer mass. Since actual masses usually are higher than the nominal integer mass due to isotope contributions, this sometimes results in mass miss-assignments. An Integer-Mass Offset parameter has been added to the General Preferences dialog to allow users to compensate for this.

Able To Smooth Profile Spectra Displays in MSDR

A "Profile Spectra" tab has been added to the Spectra Plot Preferences dialog. Users can specify whether and how to smooth displayed profile spectra. They are smoothed by default.

Spectral Deconvolution

A "Deconvolute Spectrum" option is displayed in the Spectra Plots pane right-click menu when profile spectra are displayed and the Mass ID[™] spectral deconvolution application has been installed. Selecting it will export the current spectrum to the spectral deconvolution application.

New Compound Identification Acceptance Criteria

RRT% Deviation and Peak S/N Reject have been added as new Compound Identification Acceptance Criteria. Their specification parameters are presented along with the existing Ion Ratio parameters in a new "Compound Confirmation Criteria" group box in the Calculations Setup dialog. The existing "Report Ion Ratio Outliers As [Failed|Missing]" method parameter has been generalized to apply to the new acceptance criteria as well, and the label has been changed to "Report Outliers As". Compound-specific Peak S/N Threshold values are specified on the Compound Table Integration tab.

Quantitation applies the specified acceptance criteria to "identified" compounds (peak in Search Window has been detected, integrated area/height passes Peak Size Reject specification, it passes Mass Threshold specification if Search Type = Spectrum, and it passes the Compound Report Threshold specification) for confirmation in the same way that Ion Ratios currently are done. All specified acceptance tests will be done even if one or more of them fails. They are grouped together in Sample reports as an indented block for each compound result, in the same format that Ion Ratio results currently are reported.

Custom Reports and Autolink Actions When Processing In MSDR

An Auto-Link checkbox has been added to the "Processing Rules" in the Process View. When it is checked, Varian-supplied Custom report templates (.SWT files) and other Auto-Link applications (.EXE files) that are specified in a recalc list will be executed during processing in MSDR. Please note that the following Auto-Link applications will not be executed from a recalc list processed by MSDR: Echo.Exe, Goto.Exe, MailLink.Exe, and Wait.Exe.

New Columns Added To Results List Pane

The following user-selectable columns have been added to the Results List pane. They have not been added to MS Standard reports, such as Sample and Compound reports.

- Sample Notes
- Calibration Amount
- Multiplier
- Divisor
- IS Factor
- RF/RRF
- Amount
- Deviation Amount
- Deviation Curve
- IS Deviation

Specify Line Thickness When Printing/Exporting Calibration Curves

A Calibration Curves tab has been added to the Report Preferences dialog to allow users to specify line thickness when calibration curves are printed or exported.

Specify Scientific Notation in Results

A Scientific Notation tab has been added to the General Preferences dialog to allow users to specify a threshold for reporting results in scientific notation, or to disabled it completely.

Suppress Print Date on Printed Reports

A Misc tab has been added to the Report Preferences dialog to allow users to suppress the print date on printed reports.

Add Compounds to Method

Compounds now can be added to a method compound table from the Plots View and Library Search a Spectrum windows via new right-click menu options in the spectrum panes. When added from the Search spectrum pane, the identification information for the currently selected match will be included in the added compound table entry. Compounds are added to an existing data handling section for the ms detector type of the data file that the spectrum was selected from.

Calculate Chromatogram Time Range

A Calculate Time Range option has been added to the Chromatogram Click & Drag toolbar icon, and an 'r' Hot-Key also has been added. The time in seconds will be displayed for the dragged chromatogram region or peak.

CORRECTIONS

MSDR Plots View Id: 3741 Title: MSDR: Can't edit user library entries Component: MS Workstation Platform Area: MSDataRev - LibManager, NIST

	Description:	When a spectrum from a user library is edited, clicking the Save button in the edit dialog now automatically saves the edited version of the spectrum back to the library.
ld: 3805	Title:	Name Search in MSDR and NIST return different results
	Component:	MS Workstation Platform
	Area:	MSDataRev - LibSearch, NIST
	Description:	A library Name Search in MSDR did not always return the same
		results that were returned when the same search was done in NIST. Updating to NIST 05 eliminates the discrepancy.
ld: 4005,	Title:	Hard to select .RUN files in Plots View
5008	Component:	MS Workstation Platform
	Area:	MSDataRev - MultiChro Display
	Description:	Previously, the following had to be done in order to display .?MS and .RUN files simultaneously in the MSDR Plots View:
		 Select the first file in the Data Files pane for display, and then select the desired plot descriptor(s).
		2. Select the second file in the Data Files pane via Ctrl+Click.
		 Select the desired plot descriptors for the new file via Ctrl+Click.
		The selection and display of .RUN files has been improved.
		 Chromatograms for both .RUN files and .?MS files are displayed immediately when the files are selected in the Data Files pane via Ctrl+Click.
		 RUN files now also can be selected in the Select Files dialog or by double-clicking on them in MS Explorer.
		Attempting to load a .RUN file into the Process or Results views now displays a warning message.
		Caveat: The Plot Descriptors pane displays the descriptors that are available in the last file that was selected. Since descriptors in .RUN and .?MS files are very different, the displayed descriptors won't be appropriate for all of the selected files when both types are selected at the same time.
	Title:	Zoomed spectrum mass range doesn't stick
ld: 4030	Component:	MS Workstation Platform
	Area:	MSDataRev - MultiChro Display
	Description:	Now when the spectrum display is zoomed, it will stay zoomed when
	Decemption	a different file is clicked on and the spectrum display is updated, regardless of the spectra display specifications in the Preferences dialog.
Id: 4070	Title:	Quick Integration Display Problems
ld: 4079, 4820	Component:	MS Workstation Platform
4020	Area:	MSDataRev - MultiChro Annots
	Description:	1) Previously, when Quick Integration was done on a chromatogram,
		the display only filled in the first 500 integrated peaks. Now there is no limit.
		 The Quick Integration chromatogram display was not updated when no integrated peaks were found after re-integrating.
		3) The "Noise Type Used" in the Quick Integration results display was not updated when no integrated peaks were found after re-integrating.

ld: 4536	Title:	Expansion of Data Files Pane loses displayed context information
	Component:	MS Workstation Platform
	Area:	MSDataRev - MultiChro Display
	Description:	Previously, when a directory or recalc file was expanded in the Data Files pane and there were more files than can be displayed in the pane, the display shifted to the bottom of the expanded list and to the right to display the end of the longest filename. As a result, the display context was lost. Now expansion displays the top-left portion of the expanded list.
ld: 4617,	Title:	MSDR: Improve the Quick Integration Results dialog display
4766, 4820	Component:	MS Workstation Platform
	Area:	MSDataRev - MultiChro Display
	Description:	The following changes have been made to the Quick Integration Results dialog:
		 A "% of Total" column has been added to the displayed results in the Quick Integration dialog.
		The results now display the source of the integration parameters that were used.
		 The Integration parameters have been regrouped for more clarity, and a "Use RMS Noise Calculation" checkbox has been added.
		 The "Lock Peak Width" parameter now is active only when "Use Local Parameters" is selected.
ld: 4768	Title:	Quick Integration can miss peaks on segment breaks
	Component:	MS Workstation Platform
	Area:	MSDataRev - MultiChro Display
	Description:	Previously, Quick Integration did not integrate peaks that crossed a segment boundary.
ld: 4787	Title:	MSDR: Chromatograms made from Spec Pane aren't deleted correctly
	Component:	MS Workstation Platform
	Area:	MSDataRev - Chromat. Selection
	Description:	Chromatograms can be created from a displayed spectrum via single- click and click-and-drag mouse actions, and also by accumulating multiple selections in a dialog. Previously deleting one of the extracted chromatograms could delete other chromatograms instead If the chromatogram that they were extracted from, ie, the chromatogram that the spectrum is from, was deleted, all of the extracted chromatograms were deleted.
ld: 4833,	Title:	Export Spectrum To Nist Limited by User Rights
5166	Component:	MS Workstation Platform
	Area:	MSDataRev - LibSearch, NIST
	Description:	Previously, spectra could not be exported to NIST by users with Power or Limited User rights.
ld: 4844	Title:	Noise calculations still are segment-based
	Component:	MS Workstation Platform
	Area:	MSDataRev - General
	Description:	Previously, interactive and Quick Integration Noise calculations were constrained to the segment that contained the selected point or integrated peak for which S/N calculations were being done. This could result in very large Noise values if the segment was very small

		and/or did not contain any baseline region.
ld: 4850	Title:	Add " Active Chromatogram" to target list search options
	Component:	MS Workstation Platform
	Area:	MSDataRev - LibSearch, Chrom
	Description:	Now users can select "Active Chromatogram" when "Target List
		Search a Chromatogram" is selected from the application Search
		menu
ld: 4857	Title:	Target List Search Ctgm doesn't find small peaks
	Component:	MS Workstation Platform
	Area:	MSDataRev - LibSearch, NIST
	Description:	Previously when Target List searching a chromatogram, peaks smaller than 1% of the maximum chromatogram amplitude could not be identified. The minimum height specification has been changed from 1% to 0.01% of the maximum amplitude.
ld: 4872	Title:	Change Search menu "Select Search Libraries" to "Library Manager"
	Component:	MS Workstation Platform
	Area:	MSDataRev - LibManager, NIST
	Description:	The text of the "Select Search Libraries" option in the application Search menu has been changed to "Library Manager".
ld: 4929	Title:	Spectrum averaging is segment-based
	Component:	MS Workstation Platform
	Area:	MSDataRev - MultiChro
	Description:	Previously, an averaged spectrum could not be generated and
		displayed for chromatogram points that cross a segment break if the
		instrument conditions used to collect the scans were not identical for
		all of the scans.
ld: 4940	Title:	Scan Time needs to be removed from Long Descriptor
	Component:	MS Workstation Platform
	Area:	MSDataRev - General
	Description:	MSDR determines whether two scan functions in different segments are the same by comparing the long descriptors. Since Quad data contained the Scan Time in the long descriptor, the same scan function in adjacent segments was "different" if different numbers of scan functions were specified in each segment. In this situation, the same scan function was listed separately for each segment, they produced separate chromatograms, and a compound that crossed the segment boundary could not be quantitated. This has been fixed by removing the Scan Time from the long descriptor.
ld: 5009	Title:	Problems loading files from outside MSDR
	Component:	MS Workstation Platform
	Area:	MSDataRev - Chromat. Selection
	Description:	If MSDR was open but the Plots View was not displayed when a file
		was double-clicked on in MS Explorer or MSDR was invoked from System Control, the Plots View was created but remained blank. This
		was a side-effect of other changes that were made in 6.6. It worked
		correctly in 6.5.
ld: 5011	Title:	Display problems when all Views are closed
iu. 3011	Component:	MS Workstation Platform
	Area:	MSDataRev - Chromat. Selection
	Description:	Users now are prevented from closing the Plots, Process, and Results
		Views via the 'x' box, since closing the views can cause various

		display inconsistencies. The View icons on the application toolbar should be used to access the desired view.
		Caveat: The Process and Results Views still will be closed when the 'x' box is clicked on if the user has not already clicked somewhere in the view.
ld: 5022	Title:	Plot Descriptors Pane does not list User Traces
	Component:	MS Workstation Platform
	Area:	MSDataRev - General
	Description:	Previously, User Traces were not displayed in the Plot Descriptors pane by default. This sometimes caused confusion for Quad users. The Plot Descriptors tab specifications in the Plots View Preferences dialog have been changed to display User Traces by default.
ld: 5147	Title:	Real time chrom in MSDR displays phantom scan points in addition to merged TIC
	Component:	500-MS
	Area:	MSDataRev - General
	Description:	Previously, when real-time TIC chromatograms were displayed in MSDR for multi-channel data, points were displayed for the individual scan functions in addition to the Merged point. No spectra would be displayed when these points were clicked on. Now, the last displayed Merged chromatogram point in the real-time chromatogram is updated as each individual scan in the scan function cycle is acquired
ld: 5183	Title:	Deleting "Dual-Scale" chromatogram crashes MSDR
Iu. 5105	Component:	MS Workstation Platform
	Area:	MSDataRev - MultiChro Display
	Description:	Previously, when a .RUN chromatogram and an .XMS chromatogram were displayed together as Dual Scale (= Overlaid when the units for the two chromatograms aren't compatible) and one of the chromatograms was deleted via the 'x' box, MSDR could crash.
ld: 5270	Title:	All 500-MS User Traces labeled "Ion Time"
10: 5270	Component:	MS Workstation Platform
	Area:	MSDataRev - MultiChro Display
	Description:	"Ion Time" was displayed as the y-axis label for all 500-MS User Trace plots.
ld: 5301	Title:	Chromatograms show segment gaps if different channel lists
	Component:	MS Workstation Platform
	Area:	MSDataRev - MultiChro Display
	Description:	Scan function chromatogram traces displayed gaps between segments if the plotted scan function was not on the same physical channel in each segment.
ld: 5302	Title:	Selecting data file in MS Explorer doesn't update Data Files Pane
	Component:	MS Workstation Platform
	Area:	MSDataRev – Chromatogram Selection
	Description:	Previously, when a data file was selected into an already running MSDR from an outside application such as MS Explorer, the chromatogram would be added to the existing displayed chromatograms, but the Data Files and Plot Descriptors pane displays
ld: 5332	Title:	were not updated for the new selection. Selecting TIC ctgm when Auto-Select Scan Functions crashes
		MSDR
	Component:	MS Workstation Platform

	Area:	MSDataRev - MultiChro Display
	Description:	MSDR sometimes could crash when all of the following were true: It was opened by exporting a file to it from another application such as MS Explorer, Auto-Select Scan Functions was specified, and the TIC Plot Descriptor was subsequently selected in the MSDR Plot Descriptors pane.
ld: 5486	Title:	Quick Integration dialog uses wrong Noise Type
10. 5460	Component:	MS Workstation Platform
	Area:	MSDataRev - MultiChro Display
	Description:	When "Local Parameters" integration was done in the Quick Integration dialog, the Noise Type that was used was the opposite of what was specified.
ld: 5575	Title:	Expanding directories on Memory Stick disables updating of Data Files pane
	Component:	MS Workstation Platform
	Area:	MSDataRev - Chromatogram Selection
	Description:	Previously, after the directories on a memory stick or CD were expanded in the Data Files pane, the display could no longer be updated.
ld: 5612	Title:	Can't select files in MS Explorer in some directories
10. 3012	Component:	MS Workstation Platform
	Area:	MSDataRev - Chromatogram Selection
	Description:	Previously, double-clicking on data files in MS Explorer that were on
		memory sticks, CDs, or root directories sometimes did not select them into the MSDR Plots view.
ld: 5703	Title:	Make Full Scan Descriptor Table always selectable in Plot Descriptor pane
	Component:	MS Workstation Platform
	Area:	MSDataRev - General
	Description:	Previously, the Full Scan Descriptor Table could only be selected in the Plot Descriptors pane by right-clicking on a scan descriptor. Now it can be selected by right-clicking on any type of descriptor in the pane.
ld: 5763	Title:	New Files in Recent Files list not displayed if Data Files pane not updated
	Component:	MS Workstation Platform
	Area:	MSDataRev - Chromatogram Selection
	Description:	Previously, when a data file was added to the Recent Files list by creating it in System Control or selecting it in another application, selecting it from the MSDR Recent files list would not display a chromatogram until after the Data Files pane display had been updated.
ld: 5771	Title:	Data Files Pane doesn't auto-update if > 500 files
	Component:	MS Workstation Platform
	Area:	MSDataRev – MultiChro Display
	Description:	Previously, automatic updating of the Data Files pane was disabled when an expanded directory that was displayed had more than data files and recalc files. This constraint has been removed since auto- updating now is disabled by default, and is much faster when it does happen.
ld: 5779	Title:	Display sub-directories first in expanded directories
	Component:	MS Workstation Platform
	Area:	MSDataRev – Chromatogram Selection

	Description:	When a directory is expanded in the Data Files pane, the sub- directories now are displayed first, to make it easier to drill down to a desired sub-directory and to be consistent with MS Explorer behavior.
ld: 5805	Title:	Garbage characters in Chromatogram Segment Titles
14. 0000	Component:	MS Workstation Platform
	Area:	MSDataRev – MultiChro Display
	Description:	The Segment Titles in chromatogram plots sometimes could be displayed incorrectly if the Chromatogram pane was too narrow.

MSDR Process View/Method Editor/Quantitation

ld: 4493	Title:	Problems processing multi-method recalc lists
10: 4493	Component:	MS Workstation Platform
	Area:	MSDataRev - Quan Recalc Lists
	Description:	If no method is specified in "Method File" field, MSDR now attempts to get it from the currently selected recalc file. When multiple methods are specified in a recalc file, MSDR now validates each data file in the list against the method that will be used to process it.
ld: 4885,	Title:	Incorrect Noise Calculations for Quantitation
5487	Component:	MS Workstation Platform
	Area:	Quan MS - General
	Description:	Previously, Noise calculations used by quantitation to detect peaks and report Peak S/N values were constrained to the segment that contained the Method Retention Time. This could result in erroneous values and unreliable peak detection if the peak crossed segment boundaries or spanned the entire segment.
ld: 5077	Title:	Problems locking calibration data in method
	Component:	MS Workstation Platform
	Area:	DHMeth MS - Results Treatment
	Description:	Previously, the following problems happened when the user attempted to lock calibration data in the Results Treatment dialog in the method editor:
		 Changing the "Replicates Addition Rule" to "Never Add" deleted existing calibration data.
		 When calibration data was locked via the "Edit/Lock Coefficients" dialog, the "Method & Results not the same" dialog would be displayed when the files were subsequently loaded into the MSDR Results View.
ld: 5123	Title:	Incorrect "Too few data points" msg prevents quantitation
10.0120	Component:	MS Workstation Platform
	Area:	Quan MS - Cmpd Quantitation
	Description:	Previously, when a Target Compound Integration Window crossed a data file segment boundary, quantitation couldn't be done if the segment that contained the Compound Method RT didn't contain enough points in the Integration Window, even if there were enough points in the window across the two segments.
ld: 5124	Title:	Cmpd Quantitation across segment boundaries sometimes fails
	Component:	MS Workstation Platform
	Area:	Quan MS - Cmpd Quantitation
	Description:	Quantitation can fail if all of the following are true:
		1. The peak crosses a data file segment boundary.
		The peak retention time is in a different segment from one run to the next.

		 The Compound Method RTs are updated automatically when calibration files are processed.
		 The scan functions that are specified for quantitation are on different physical channels in each segment.
		To prevent this from happening, set "Update Compound Method RTs" to "No" in the Results Treatment dialog in the method editor. This ensures that the Method RT will not move to a different data file segment.
		Note: Quantitation still could fail if the scan function being used to generate the chromatogram was on different physical channels in the adjacent segments, and the total number of channels in the other segment was less than the channel number that the scan function was on in the segment that contained the compound Method RT. This has been fixed.
ld: 5125	Title:	Problems when changing Cmpd RT to different segment in editor
	Component:	MS Workstation Platform
	Area:	DHMeth MS - Compound Table
	Description:	Previously, the scan function specification used to display the
	Description.	compound chromatogram in the method editor became incorrect when the compound RT was changed on exiting the Compound Attributes or Quan Ions tab of the Compound Table if all of the following were true:
		 The Integration Window crosses a data file segment boundary.
		2. The Method RT is changed to a different segment by clicking on the chromatogram or typing a new RT.
		 The specified scan function is on a different physical channel in the other segment.
ld: 5198	Title:	Compound Spec Identification of combined-channel chromatograms crashes quantitation
	Component:	MS Workstation Platform
	Area:	Quan MS - Cmpd Identification
	Description:	Previously, quantitation sometimes crashed when compounds were identified by Spectrum Match and multiple scan functions were combined into a single chromatogram.
ld: 5254	Title:	Integration problems caused by invalid Compound Time Events
	Component:	MS Workstation Platform
	Area:	Quan MS - Cmpd Identification
	Description:	Forced Peak time events that were outside of the compound Integration window could cause invalid integration results. This could cause compounds to be inappropriately reported as Missing, and could cause Custom Reports to close. This was caused by a problem in the 6.5 software with the graphical Time Events bar in the Integration pane. Time events that were specified for a compound could be saved back to multiple compounds in the permanent
		method. This was fixed in 6.6, but existing methods still could cause problems. In 6.7, the inappropriate Time Events are ignored during quantitation.
ld: 5469	Title:	Method Editor discards changing Quan Ion specification to RIC
	Component:	MS Workstation Platform

	Area:	DHMeth MS - General
	Description:	When a numeric Quan Ion specification was changed to RIC, the
		editor sometimes discarded the change.
ld: 5617	Title:	MSDR doesn't respond during processing when cpu = 100%
	Component:	MS Workstation Platform
	Area:	Quan MS - General
	Description:	When the CPU load during quantitation was very high, other user actions such as clicking on the Cancel button or displaying a dialog from another application on top of the Process View could cause MSDR to not respond until quantitation of the current file was complete. The screen would not be re-painted, the application title bar would display "not responding", and the Cancel request would often be ignored even after quantitation of the current file finished.
ld: 5659	Title:	Compound Table Header Text is clipped
	Component:	MS Workstation Platform
	Area:	DHMeth MS – Compound Table
	Description:	The bottom of the text in the Compound Table column headers is missing.
ld: 5780	Title:	Can't scroll past compound window boundaries in compound table chromatograms
	Component:	MS Workstation Platform
	Area:	DHMeth MS – Compound Table
	Description:	Previously, the compound chromatogram display could not be scrolled past the compound window boundaries.
ld: 5796	Title:	Quantitation hangs in rare Time Events situation
	Component:	MS Workstation Platform
	Area:	Quan MS – Compound Quantitation
	Description:	Previously, Compound quantitation could hang if all of the following were true: 1. Spec Match identification
		 There is a Group Peaks Time event whose start time is <= the Integration Window Start Time & end time is >= the Integration Window End Time.
		 There are integrated peaks in the Search Window that pass the specified Peak Size Reject Threshold, but nothing passes the Match Threshold.

MSDR Results View/MS Standard Reports

ld: 3865	Title:	Analysis results outside cali range not shown on curve
	Component:	MS Workstation Platform
	Area:	MSDataRev - General
	Description:	Previously, an analysis result that was outside the calibration curve range was not shown on the curve when it was a log plot.
ld: 4674	Title:	MSDR: Print Calib Curve Reports from Results View not working
	Component:	MS Workstation Platform
	Area:	MSDataRev - Reports, View&Print
	Description:	Printing and exporting from the Results View use the "Preview Reports" and "Print to Spooler" specifications in the application File menu. If Print to Spooler was selected and Preview Reports was not selected, reports were sent directly to the spooler file with no indication of what was happening. Now, an action status message is

		displayed.
ld: 4753	Title:	In Single data file results view, calibration points exclusion is not remembered
	Component:	MS Workstation Platform
	Area:	MSDataRev - General
	Description:	Previously, Exclude/Include calibration point changes were discarded when a different data file was selected and the Results List pane was configured to display results for a Single Data File only:
		 Changes in the Point Info dialog did not accumulate when different points are selected in the dialog.
		Changes did not accumulate when a different data file is selected in the Study or Results List panes.
		3. Right click changes in the pane did not accumulate.
ld: 4861	Title:	Can't Print Summary Reports from Results View
	Component:	MS Workstation Platform
	Area:	MSDataRev - Quan, Review Results
	Description:	Previously, the Summary and Chart reports were not available for selection when users clicked on the Print button in the MSR Results view.
ld: 4952	Title:	Analysis result on cali curve not adjusted for Cmpd Multiplier
	Component:	MS Workstation Platform
	Area:	MSDataRev - Quan, Review Results
	Description:	When Analysis results are displayed on the calibration curve, the Multiplier and Divisor from the recalc list are factored out so that the
		result will intersect the curve. Previously, the Compound Multiplier
		from the method was not factored out. If the Multiplier or Divisor does
		not equal 1.0, a dashed vertical line is displayed to show that the
		Amount from the curve is different from the calculated Amount.
ld: 4953	Title:	Clicking on compound or file in Study pane doesn't always select
	Component:	MS Workstation Platform
	Area:	MSDataRev - Quan, Review Results
	Description:	When compounds or data files were clicked on in the Study pane in the Results View, and then a different result was selected in the
		Results List pane or the Calibration curves pane, the selection "***" marker in the Study pane was updated but the gray hi-light was not. When the hi-light was clicked on again, nothing happened because it was out of sync with the "***" marker. Now they are updated together.
ld: 4986	Title:	Problem exporting Amount in Summary Reports
10. 4500	Component:	MS Workstation Platform
	Area:	MSDataRev - Reports, View&Print
	Description:	Previously, the calculated result and the units were combined into a
		single "Amount" column when Summary reports were exported to an ASCII file. This caused problems when importing the file into Excel.
ld: 5014	Title:	Click & Drag integration not saved to method
-	Component:	MS Workstation Platform
	Area:	MSDataRev - Quan, Review Results
	Description:	When a calibration result was modified by Click&Drag integration and
		the changes were saved to the permanent files, they were not saved back to the calibration curves in the method unless some other change that modifies the method also was made before saving the changes.

ld: 5015	Title:	Calibration curve changes not saved to method
	Component:	MS Workstation Platform
	Area:	MSDataRev - Quan, Review Results
	Description:	When the Curve Point, Origin Point, or Regression Weighting parameters were changed via the right-click menu in the Calibration Curves pane, the Process button were clicked on and the changes were saved back to the permanent files, the curve parameter changes were saved back to the method calibration data, not to the method specification parameters. As a result, reprocessing the files with the method wiped out the "saved" method changes.
ld: 5040	Title:	Reprocessing in Results View deletes RRT values
	Component:	MS Workstation Platform
	Area:	MSDataRev - Quan, Review Results
	Description:	Previously, reprocessing in the Results View deleted existing RRT values.
ld: 5135	Title:	Can't load "compatible" single data file into Results View
	Component:	MS Workstation Platform
	Area:	MSDataRev - Quan, Review Results
	Description:	When files are loaded into the Results View, a dialog is displayed if the method and data file results are not consistent. This can be overridden if the method and data files are compatible (the differences do not invalidate the calibration data) by checking the "Use With All Compatible Files" checkbox. However, the Compatible Files checkbox was disabled if a single data files was being loaded into the Results View rather than a recalc file.
ld: 5141	Title:	No Spectrum info for some Missing peaks
	Component:	MS Workstation Platform
	Area:	MSDataRev - Quan, Review Results
	Description:	Previously, a Sample spectrum was not displayed in the results for a Missing compound if identification was not by Spectrum Match, or if no peaks were detected and passed the Peak Size Reject threshold. Now a spectrum is always displayed, both in the MSDR Results View Spectrum pane and in the Compound reports. If the compound is Missing and an Actual Retention Time is not available, the spectrum for the Method Retention Time will be displayed.
ld: 5196	Title:	Click & Drag manual integration displays wrong area value
	Component:	MS Workstation Platform
	Area:	MSDataRev - Quan, Review Results
	Description:	Previously, Click & Drag integration displayed an area on the chromatogram that was slightly different from the area reported in the results. This area was calculated by the peak "fill-in" drawing mechanism, and may not be the same as the actual integrated area. It has been eliminated.
ld: 5268	Title:	Quan S/N calculations wrong if peak height greater than 200000000
	Component:	MS Workstation Platform
	Area:	MSDataRev - Quan, Review Results
	Description:	Previously, the S/N values that were reported for Target compounds were wrong if the peak height was greater than 2000000000. They were correct for Unknown peaks.
ld: 5282	Title:	Cali Curve pane: no right-click menu items for internal standard compounds
	Component:	MS Workstation Platform

	Area:	MSDataRev – Quan, Review Results
	Description:	The Calibration Curves pane did not display the right-click menu if the current compound was an internal standard.
ld: 5451	Title:	Some numeric columns not right-justified in Results List reports
	Component:	MS Workstation Platform
	Area:	MSDataRev – Quan, Review Results
	Description:	Some numeric columns in the Results List pane were not right- justified in the printed reports.
ld: 5463	Title:	Accessing Results View can crash if Compound Table empty
	Component:	MS Workstation Platform
	Area:	MSDataRev – Quan, Review Results
	Description:	MSDR could crash when going to the Results View if the files were processed as %, the method Compound Table was empty, and the Results View Preferences dialog specified to just display results for a Single Compound.
ld: 5488	Title:	Increase reported RRT results from 2 decimal places to 3
14. 0100	Component:	MS Workstation Platform
	Area:	MSDataRev – Reports, View & Print
	Description:	RRT results now are reported to three decimal places.
ld: 5770	Title:	Speed up creation of Sample and Compound Reports
	Component:	MS Workstation Platform
	Area:	MSDataRev – Reports, View & Print
	Description:	The creation of Sample and Compound reports now is faster.

MSDR General/Miscellaneous

	MSDR General/Miscellaneous		
ld: 3886	Title:	MSDR: Method not remembered after switching views	
	Component:	MS Workstation Platform	
	Area:	MSDataRev - General	
	Description:	Previously, a previous method selection was discarded when entering the Process View if it was different from the method that was used to process the files, or if the files had not been processed. Now the selection is remembered. The user can choose which method to use if it is different from the one that was used to process the files.	
ld: 4788	Title:	Problems accessing Process & Results Views with profile file	
	Component:	MS Workstation Platform	
	Area:	MSDataRev - General	
	Description:	Accessing the Process or Results View with a profile data file or selecting one while in the view now displays a warning message.	
ld: 4934,	Title:	No vertical scale in System Control plots if no intensities	
4941	Component:	MS Workstation Platform	
	Area:	ModWin - Acquisition	
	Description:	In System Control, the vertical scale was not displayed in the Chromatogram and Spectrum plots if there were no intensities.	
ld: 5016	Title:	Quadrupole Log File Display	
	Component:	MS Workstation Platform	
	Area:	MSDataRev - Reports, View&Print	
	Description:	The tree display for quad files in the log info dialog has been re- organized and simplified.	
ld: 5083	Title:	Data file not always added to Most Recent list	

	Component:	MS Workstation Platform
	Area:	MSDataRev - Chromatogram Selection
	Description:	When a data file was loaded into an already-running MSDR by double-clicking on it in MS Explorer, it was not added to the Most Recent Data Files list. It was added if MSDR was not already running.
ld: 5129	Title:	Adjust 500-MS Mass Centroiding
	Component:	MS Workstation Platform
	Area:	DAMeth - General
	Description:	Mass centroiding has been adjusted for the improved Fast scan speed mass resolution, and to handle multiply-charged ions in both Fast and Normal scan speeds.
ld: 5139	Title:	Move MSDR .ini files to VarianWS directory
	Component:	MS Workstation Platform
	Area:	MSDataRev - General
	Description:	The MSDR .ini files have been moved to the VarianWS directory from the Window directory. Some users may not have access to the Windows directory.
ld: 5205	Title:	Scrollbars cause crash in System Control Chromatogram Display
	Component:	MS Workstation Platform
	Area:	System Control - Acquisition
	Description:	The horizontal scrollbar was sometimes displayed for the first few points in an acquisition when it should not be. Using it could cause a crash.

Custom Reports Changes

ld: 3281	Title:	Header on Every Page for Multi-Compound Basic Report Template
	Area:	Multi-Compound Basic Custom Report
	Description:	The Multi-Compound Basic Report now can optionally print a header on each page of the report instead of a header on just the first page. A checkbox on the report's file selection dialog allows the user to choose between a header on each page or only on the first page of the report.