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

Varian MS Workstation Version 6.5 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 6.5
- Items of Interest to Users Upgrading from MS Workstation Version 6.42 (and earlier)

All Varian MS Workstation operators should read the section "Items of Interest to All Users of the Varian MS Workstation Version 6.5."

Customers upgrading an existing system should read "Items of Interest to Users Upgrading from MS Workstation Version 6.42 (and earlier)."

Items of Interest to All Users of the Varian MS Workstation Version 6.5

General Operational Considerations

System performance in general, and Quantitation in particular, can be seriously degraded if the PC has a slow CPU (<500 MHz), less than 512 MB RAM, anti-virus software is enabled, or other software that may compete 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.

The minimum supported screen resolution for the Workstation software is 1280 by 1024. In this release, some of the dialogs have been enlarged and the layouts have been enhanced to take advantage of this greater minimum resolution.

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.

Ensure that your computer meets the Minimum Computer Requirements listed below:

- Operating System: Windows 2000 or XP Professional. Windows 98 is supported for Saturn 2000 users only. Windows NT 4.0 (with service pack 6) is supported for Saturn 2000 or 1200 MS users only.
- Pentium III (or higher) processor, at least 500 MHz, or greater.
- Video screen supporting 1280 x 1024 x 256 resolution or greater. 16-bit color is recommended.
- At least 512 Megabytes RAM
- CD-ROM drive, 16X or faster

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 a Windows NT, 2000, or XP system. (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 6.5 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 6.5, serial numbers from pre-6.5 versions of the core MS Workstation software will not work with 6.5. You must purchase an upgrade to use the MSWS 6.5 software.

Update Ver 6.x to Ver 6.5 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 6.5, serial numbers from pre-6.5 versions of the core MS Workstation

software will not work with 6.5. You must purchase an upgrade to use the MSWS 6.5 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 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.

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 6.5 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.

MS 1200 DRIVER

The MS 1200 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 1200 is present or not. If you do not plan to connect a 1200 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 WS 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

MS Data Review implements an "Explorer-like" interface that allows you to browse Workstation files. The directory tree in the Data Files pane is updated every few seconds to reflect changes to the tree, such as adding, moving, or deleting data files or recalc list files, or adding or removing memory sticks. When a directory containing large numbers of files is displayed, this updating can cause the response to user actions to be delayed for several seconds. Therefore, automatic updating of directories that contain more than 500 data files is only done about every 30 minutes. These large directories can be updated manually at any time by selecting the "Update Floppy and Network Drives on File Tree" option in the application View menu.

Accessing directories in the Plots View Data Files pane that contain large numbers of data files can affect the performance of MS Data Review. For optimum performance, directories should not contain more than 1,000 data files.

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, MS Data Review can be started in the following ways:

- 1) Click "Start" on the Windows Task Bar, select Run..., enter "\VarianWS\msdr5.exe -3", and then click on OK. This will change the "File to Display on Start Up" specification in the Application Start Up Preferences to "None", and then start the application.
- 2) If the "File to Display on Start Up" specification in the Application Start Up Preferences was "Last Data File", open another MS Workstation application and select a valid MS file. If the Preferences specification was "Last Recalc File", open the Automation File Editor and select a different recalc file. When MS Data Review is started, it will auto load the valid file.

Items of Interest to Users Upgrading from MS Workstation Version 6.42 (and earlier)

Introduction

WHAT'S NEW

The most significant changes made in 6.5 are to the MS Data Review Application. An optional file browser was added to the Qualitative Plot Window and a new integrated Results Window allows results to be browsed, reviewed, and updated more conveniently. See the MS Data Review section below.

This release also contains some changes to the core Workstation, including the latest updates to the rest of the components of the MS Workstation.

GENERAL CHANGES

Beginning with the previous (6.42) release, the STAR32.INI file that contains some of the persistent configuration information for the MS Workstation was moved from the Windows directory to a System subdirectory of the Workstation installation directory. This eliminated problems occurring when the current user did not have rights to modify this file in the Windows directory.

To install the Workstation, the current Windows user must have administrative rights. To use the WS, the current Windows user should be at least a Power User on the local Computer. Under Windows XP, this can be set up from the "Manage" menu command in the right-click menu of the "My Computer" desktop icon.

USE OF MS ACCESS-BASED TEMPLATES

Due to a number of changes made in Version 6.X, MS Access-based templates made with previous Saturn GC/MS Workstation versions of the software are incompatible with this release. All .SWT files made with such releases should be deleted when this version is installed. In order to generate reports from pre-existing data files with new templates, the data files must be reprocessed using methods that have been built or converted with this release.

New Features of the Varian MS Workstation and Data Handling

MS DATA REVIEW

MS Data Review has been substantially revised to make it easier, faster, and more intuitive for users to accomplish their tasks in the MS Workstation. Refer to the Software Reference Manual and to the On Line Help for more detailed information.

- The number of windows, dialogs, and steps required to accomplish tasks has been reduced.
- The menus, toolbars, and bitmaps have been re-worked to make them simpler and more intuitive.

- Wherever possible, the application will load and display the desired data automatically. The application start-up and display conditions, and what data to load and display automatically, are customizable.
- Chromatograms are specified and created based on the scan functions that were used to acquire the data, rather than the channel numbers that they happen to be on.
- You can easily select, view, and reprocess information of interest across data file sets as easily as within a single data file.
- Related information is displayed in linked panes that update automatically when a selection or action is performed in any of the panes.

Printing and Export capabilities have been expanded.

- Reports can be generated, previewed, and printed during reprocessing in MS Data Review. All Standard MS reports can be viewed and printed interactively.
- Users can export the following to the Clipboard or to a Picture file: the active Chromatogram or Spectrum plot, the contents of the Chromatogram, Spectrum, or Calibration Curve panes, a click-and-drag region of a Chromatogram or Spectrum pane, the Active View, or all displayed Views.
- 3rd party PDF utilities can be used to print to PDF files.
- When chromatograms and spectra are printed or exported to a Picture file, users can specify the desired line thickness.

The previous MS Data Review windows and dialogs have been combined into 3 main views which can be directly accessed via icons on the Application Toolbar: Plot Chromatograms and Spectra, Process Data, and View Results. The existing Search windows and dialogs have not been changed, but they now are accessed via a single Search Spectra icon on the Application Toolbar.

Plots View

The Plots View combines the previous Chromatogram and Spectrum windows into a single view. New Data Files and Plot Descriptors panes have been added which allow the easy selection and display of chromatograms from entire data file sets as easily as from a single data file, and without having to go to the Select Files dialog. The Select Files dialog still exists for backwards compatibility. Chromatograms are generated from the scan functions used to acquire the data, not arbitrary channel numbers.

Multiple data files and plot descriptors can be selected in the Data Files and Plot Descriptors panes. One chromatogram will be displayed for each data file – plot descriptor association.

The display characteristics and behavior of the panes in the Plots View can be customized via the Plots View Preferences dialog. The Show/Hide icon on the Application Toolbar can be used to display the Data Files and Plot Descriptors panes for chromatogram selection, or hide them to display the chromatograms and spectra full-screen.

• Data Files Pane

The Data Files pane displays a directory tree which is similar to a standard directory tree, except for the following:

- Recalc List files are displayed and handled like directories. Directories are displayed as yellow folders, and recalc files are displayed as green folders.
- The data files in a directory or recalc list are displayed directly in the tree.

A data file in a directory that is also specified in a recalc list file in the same directory will be displayed twice: once in the directory list of files, and once in the recalc file list. A generic "file" bitmap is displayed for the file names the directory list. The bitmaps for the same files in a recalc file list also display the Sample Type.

A data file or recalc list file is selected by clicking on it, using the Up/Down Arrow keys, or via the Recent Files button. When a recalc file is clicked on, summary information for the recalc list is displayed in the Plot Descriptors pane. When a data file is clicked on, the scan descriptors that are available in the file are displayed in the Plot Descriptors pane. Multiple files can be selected via the <Ctrl>+Mouse Click combination. All of the files in the current directory or recalc file can be selected via the right-click menu.

Recalc list files can be created or modified, and the selected files or all of the files in the current directory can be added to a recalc list file via the right-click menu.

- **Plot Descriptors Pane**

The Plot Descriptors pane displays the descriptors that are available for the currently selected data file(s). A descriptor is selected by clicking on it or by using the Up/Down Arrow keys. Multiple descriptors can be selected via the <Ctrl>+Mouse Click and <Shift>+Mouse Click combinations. All of the displayed descriptors can be selected via the right-click menu.

All data files contain a TIC and 1 or more Scan Function descriptors per acquisition segment. They also may optionally contain User-Defined descriptors (described below) and User Trace descriptors (non-detector signals that may be stored by some detector types). If a data file has been quantitated, it also contains the Method descriptors that were used to quantitate the data. Each descriptor type is distinguished by a unique bitmap that is displayed to the left of the descriptor.

- **Chromatogram Pane**

The Chromatogram pane adds the following enhancements to the capabilities of the Chromatogram windows in the previous MS Data Review application:

Calculate Noise - Either Peak to Peak or RMS noise can be calculated. The Noise Type that is specified in the Chromatogram Plot Preferences dialog will be used.

Reference Chromatograms - Make the file for the active chromatogram a Reference File. Its chromatogram(s) are locked at the top of the Chromatogram pane. Other data files can be selected and the corresponding chromatograms compared to those of the Reference file.

Extract Chromatograms - Chromatograms can be extracted from the active chromatogram by typing the desired ion(s) into the "Ions" field at the bottom of the pane and then pressing <Enter>. Any combination of masses and mass ranges can be specified. A new chromatogram will be generated by extracting the specified ion(s) from what can be generated by the descriptor for the active chromatogram.

Combine Chromatograms - Multiple descriptors can be combined into the active chromatogram by clicking on the desired descriptors while holding down the <Alt> key. The selected descriptors can be in the same or in different data file segments. A new chromatogram will be generated by combining the selected descriptors into the active chromatogram.

Saving User-Defined Descriptors - The plot specification for an extracted or combined chromatogram can be saved to the data file that it was extracted from. A user-specified descriptor label can be entered when it is saved to the file. A saved user descriptor can be selected later to display the chromatogram without having to re-enter the specification, and it can be applied to other data files. It is available for selection until the user deletes it from the file.

Full-Chromatogram vs. Single-Segment Display - The chromatogram display mode can be toggled between Full-Chromatogram and Single-Segment by toggling the "S" checkbox to the left of the "Ions:" field at the bottom of the Chromatogram pane. When Segment mode is selected, the display will be initialized to the segment in the active chromatogram that contains the cursor location. If there is no cursor location in the active chromatogram, it will be initialized to the first segment that contains a trace.

Chromatogram Navigation - When the display mode is Segment, the Chromatogram Navigation control at the bottom of the pane can be used to change the display to the Next, Previous, First, or Last segment in the data file, or to a specific segment Number. If more chromatograms have been selected than can be displayed at one time, the Chromatogram Navigation control also can be used to navigate through the chromatograms of the selected data files and plot descriptors. You can navigate through the Segments (S), Data Files (F), or Plot Descriptors (P) in the Chromatogram pane display by clicking on the appropriate button to the right of the navigation control.

Spectrum Selection and Updating - The following changes have been made to how a spectrum is selected from a chromatogram:

- When a spectrum is selected by clicking on a chromatogram, it becomes the active spectrum.
 - When the chromatogram is clicked on, the resulting spectrum can be for the point that was clicked on, or for the apex of the peak that was clicked in. This is specified on the Chromatogram Plots tab of the Preferences dialog or on the Chromatogram pane toolbar. When the selection mode is Apex, the highest apex in the search window will be selected. The size of the search window around the clicked-on point to look for an apex also can be changed. All single-click actions will use the selected spectrum: Display, Search, or Export. In addition, the corresponding point will be used when Signal/Noise is calculated.
 - Changing the data file or plot descriptor for a chromatogram updates any spectra that have been selected from it.
 - Deleting a chromatogram also deletes any spectra that were selected from it.
- **Spectrum Pane**

The Spectrum pane adds the following enhancements to the capabilities of the Spectrum windows in the previous MS Data Review application:

- Selecting and updating spectra from chromatograms is done as described above in the Chromatogram Pane section.
- The location of the Spectrum pane relative to the Chromatogram pane can be specified on the Spectra Plots tab of the Preferences dialog, or by clicking the "Rotate Plots" icon in the Application Toolbar.

Process View

The Process View adds the following enhancements to the capabilities of the Process/Review windows in the previous MS Data Review application:

- Recalc list files and single data files are processed in the same view. Recent and Browse buttons have been added to select a different data file.
- Summary Reports can be interactively viewed and printed or exported.
- All recalc list lines except for .RUN files and AutoLink lines or actions can be executed.

- Processing can be done on the entire recalc list, a selected range of lines, or the selected Sample Type(s). You can specify whether existing calibration data should be deleted at the beginning of processing, regardless of whether or not the recalc list contains a "New Calibration" line.
- Automated printing during processing can be enabled. The method specifications will be used. If automated printing is enabled, you can choose to preview the reports after the recalc list processing has been completed, and to then send all, some, or none of the reports to the printer. If No Recalculate is selected, the reports will be generated from the existing results without re-processing the files.
- Reports also can be created and viewed interactively via the Print button. The selected report will be created regardless of whether or not it is specified in the method.
- When a line in the recalc list or the Processing Status pane is double-clicked on, the Results View will be displayed. The panes will be initialized to the first result in the file that generated the clicked-on line in the Process View.

Results View

The Results View displays the results for the loaded data file or recalc list in the Study and Results List panes, and up to 4 of the following user-selected panes: Integration Chromatogram, Status Log, Compound Report, Spectra Plots, TIC Chromatogram, and Calibration Curve.

You can easily review the results for an entire data file set, accumulate manual integration or method changes for all compounds in all data files in the set, and save or discard all of the changes as a unit. Individual panes can be maximized for detailed work and then restored to their previous size. Selections or actions in any pane update the other panes.

In order to keep the method and the results consistent, you will be prompted to Save or Discard any temporary changes before leaving the Results View. If the permanent method is changed in another application while it is being used in the Results View, a message will be displayed that the current results are no longer consistent with the permanent method, and must be reprocessed.

Standard MS Reports can be viewed and printed. The report method specifications can be modified and the modified reports can be view/ and printed or exported without having to reprocess. Report method changes are saved or discarded via the Save actions described above.

• Study Pane

The Study pane is always on the left side of the Results View. It displays the method compounds for the currently loaded data file. If a recalc list is loaded, it also shows the data files in the recalc list.

The compound and data file that map to the currently selected results in the other panes are indicated by asterisks ***.

- Clicking on a different compound updates the other panes for the new compound in the current data file.
- Clicking on a different data file updates the other panes for the current compound in the new data file.
- Clicking on the "Unknowns Method" updates the other panes for the first Unknown Peak result in the current data file.

- Clicking on a different data file while the “Unknowns Method” is selected updates the other panes for the Unknown Peak result that has the closest RT to that of the result in the previous file.

• **Results List Pane**

The Results List pane is always at the top of the Results View. The files that results are displayed for, the types of results that are displayed, and their sort order are specified in the Compound and Peak Results tab of the Preferences dialog. The results also can be sorted by increasing or decreasing value by clicking on the header of any column that shows an Up/Down arrow.

The specific results fields that are displayed can be selected via the Results List Columns tab of the Preferences dialog.

Columns can be dragged to the desired width. The new width will be retained until it is dragged again, even if the display is switched to another view and then back, or the application is closed and then re-opened.

The contents of the Results List pane can be printed via the Print button as an interactive, user-configured “Summary Report”, or exported to an ASCII file. Printed Results List reports will use any user-adjusted column widths.

• **Integration Pane**

The Integration pane adds the following enhancements to the capabilities of the Manual Integration windows in the previous MS Data Review application:

Click and Drag Integration - True Click & Drag integration has been incorporated into manual integration for Target Compounds. When “Integrate Area” is selected as the Click-And-Drag Mouse Mode or by holding down the “I” hot-key, the peak will be integrated automatically when the mouse button is released. Any pre-existing integration results will be eliminated. If the Start and/or End points of the dragged line are below the chromatogram trace, verticals will be drawn from the chromatogram. If the Start and/or Endpoints, are outside the peak, i.e., above the chromatogram trace, the line will be clipped to where it intersects the chromatogram.

A Click and Drag result can be discarded by right-clicking on the apex event of the manually integrated peak and selecting “Restore Method Integration”. The original integration results that were generated by the method will be restored.

Automatic Reprocessing - When a manual change is made by dragging a Peak Event or via Click and Drag integration, the result is re-integrated automatically when the mouse button is released. If it is a calibration data point, the compound results will be recalculated in all Analysis and Verification files.

Method changes automatically reprocess all files that are quantitated with the method when the edit dialog is OK'd. If method changes are made via the graphical Time Events bar, Process and Cancel buttons will be displayed to the left of the bar until the accumulated changes are processed or discarded.

• **Calibration Curve Pane**

The Calibration Curve pane adds the following enhancements to the capabilities of the Calibration Curve window in the existing Method Builder application:

- The location of the current Verification or Analysis result is displayed on the curve.
- The % Deviation of the current Calibration or Verification data point is displayed above the plot.

- The right-click menu is used to access the parameters, actions, sub-dialogs, etc. that are present in the existing Calibration Curve dialog.
- When calibration curve parameters, coefficients, or excluding/including calibration data points are changed, Process and Cancel buttons will be displayed in the pane. When the Process button is clicked, results in all Analysis and Verification files that use the changed curve will be reprocessed. Clicking on the Cancel button will discard the changes.

QUANTITATION IMPROVEMENTS

Most of the usability improvements are in the MS Data Review application. However, some changes also have been made in Method Builder and in quantitation to support these changes.

Improved Target Compound Identification

- Spectrum Match Identification tests are done only on integrated peaks whose apexes are in the Search Window and that exceed the Peak Size Reject Threshold.
- “Retention Time” Identification has been replaced by “Nearest, Highest, First, or Last”. “Nearest” is equivalent to the previous “Retention Time” Search Type.

Scan Function-Based Quantitation

- In the Scan Function Channels field, the Scan Descriptors are displayed instead of the Channel number.
- In the chromatogram plots on the Compound Table Entry pages, scan-function-based chromatograms and plot labels are displayed.
- The rule that constrained Target Compound chromatograms to a single data file segment when identification was by Spectrum Match has been eliminated.

Miscellaneous

- The Quan Ions can be typed directly in the Quan Ions fields in the Compound Table Quan Ions page and the Calculations Setup dialog.
- In the Calculations Setup dialog, users can specify either Peak-To-Peak or RMS noise for quantitation. P-P noise typically will be 3-5 times higher than RMS noise. The default method specification is P-P, but quantitation will continue to use RMS noise when existing methods are used without modifying them. A given set of peak detection/integration parameter specifications will generate similar results regardless of the Noise Type that is selected.
- Quantitation of Unknown Peaks now always uses “Merged”. Specifications other than Merged in existing methods will be ignored by quantitation.

CUSTOM REPORT TEMPLATES

For MS Workstation 6.5, the Multi-Compound Report application has been enhanced to allow standard chromatography .RUN file plots to be displayed and printed on reports. This feature is available for the Sample, Chromatogram, and Compound Report types.

To add a .RUN file plot to a report, edit the report template and then select the 'Configure Graphic' button. For one or more of the three chromatogram traces, select option button 'R' and then select the .RUN file to be plotted (either a fixed file name or a file name derived from the current .MS file name). By default, the first channel in the .RUN file will be plotted; to plot a different channel, enter the desired channel number into the Channel List field.

1200 MS Issues Resolved

Id: 3291	Title: Component: Area: Description:	1200 Capillary Voltage Auto Tune Problem 1200 ModWin - Auto Tune If you only tune Q3 (+), the AutoTune pml will not use the Capillary volts that are specified in the Standard Compound table. Instead it is using 200V, which is causing breakdown and lack of signal forcing the software to increase the detector voltage in trying to find the target ions.
Id: 3320	Title: Component: Area: Description:	Don't Require System Control Restart after Configuration Change 1200 ModWin - General Whenever certain items in the 1200 Configuration dialog are changed, a restart of System Control is forced.
Id: 3356	Title: Component: Area: Description:	Relocate CONFIG.CUB from the drive root to \VarianWS\1200Sys 1200 ModWin - General Since, in the new security-conscious world of Windows XP, access to the root directory of a disk cannot be guaranteed, the CONFIG.CUB file must be moved someplace else where its access can be (more or less) assured. Move CONFIG.CUB from the root directory to the \VarianWS\1200Sys subdirectory.
Id: 3368	Title: Component: Area: Description:	System errantly into Bakeout 1200 System Control - Automation System errantly went into bakeout during sample list.
Id: 3433	Title: Component: Area: Description:	1200: Hardware Diagnostics 1200 ModWin - General Display the diagnostics report at the end of running the diagnostics. There must be a reason for troubleshooting the Instrument, so let the user know the outcome of the tests.
Id: 3518	Title: Component: Area: Description:	1200: cal gas not turned off after EDR calibration 1200 ModWin - Auto Tune Execute EDR calibration on 1200 GC/MS, after it is done, filament and detector turned off automatically, but the cal gas is still on, I have to turn it off manually.

Id: 3546	Title: Component: Area: Description:	1200: SIM Width in Current Scan dialog 1200 ModWin - General The correct SIM Width range is 0.1-5.0 amu, but the Current Scan dialog can accept out-of-range values in this field. It only checks and corrects the range after it is closed and reopened. E.g. if you enter 1000amu in the field, it will not complain when you apply the entry, but when you reopen the dialog it will have 5.0 amu.
Id: 3564	Title: Component: Area: Description:	Security App doesn't work with 1200 Scan Method change 1200 ModWin - Diagnostics From the WS Security application enable the "Require revision log entry when changes to methods are saved" setting. From System Control, make a change to the 1200 Scan Method and select 'Save as Active Method'. The changes get saved without asking to add a revision log entry. From Method Builder, it works OK.
Id: 3590	Title: Component: Area: Description:	Wrong Acquisition Method is Placed in Method 1200 ModWin - Acquisition A "default" 1200 Acquisition Method is being placed in the resulting XMS file whenever an acquisition is performed. Please put a copy of the actual method that has been executed into the XMS file instead.
Id: 3601	Title: Component: Area: Description:	First scan in ESI MSMS with EDR is too large 1200 Other Using ESI with EDR on and a MSMS (311->156) method. The first scan when data collection starts is relatively high when compared to succeeding points. In one case the first point was at 9e+2.
Id: 3617	Title: Component: Area: Description:	1200 quad evaluation, calgas not on in EI mode 1200 System Control - General Cal gas should be turned on when quadrupole evaluation starts.
Id: 3620	Title: Component: Area: Description:	1200: Log entry header has clipped text 1200 DAMeth - General The 1200 scan method log header for 'Collision Energy' is clipped to read 'Collisio' . Rearrange the headers to include a 2nd line and read as: Capillary Q1FM Q1LM Q3FM Q3LM Collision CID Energy
Id: 3623	Title: Component: Area: Description:	1200: DIP probe temps don't reach setpoints 1200 System Control - General The 1200 temperature readbacks for the DIP probe are always about 5-10 degrees short of the setpoints. i.e.: setpoint : 50 ; actual : ~45 setpoint : 100; actual : cycles between 92-96 setpoint : 200; actual : cycles between 188-196
Id: 3634	Title: Component: Area:	1200: collision energy can get reordered in channels 1200 DAMeth - General

	Description:	Build a 1200 scan method with several channels. Keep the Q1 ions and Q3 ions the same and vary the collision energy in ascending order. When you save the method the collision energy order gets 'flipped' to a descending order. If you run this method and look at the log, the collision energy is in the original ascending order. But the acquisition method will still show it in descending order.
Id: 3645	Title: Component: Area: Description:	1200 workstation, release note has nothing to display 1200 System Control - General Release note under help menu in 1200 system control, is not working. It should have workstation version displayed at minimum.
Id: 3646	Title: Component: Area: Description:	set capillary in autotune does not work 1200 System Control - General In autotune, API (ESI) source, the tune-compound editor has a check box "set capillary". This should allow the user to enter desired values for the capillary voltage at each tune mass. The autotune should not optimize the capillary voltage if this option is selected. This works OK for a "factory" tune compound but does not work for a "user defined" tune compound. For a user defined tune compound, the capillary voltage is optimized, even if the "set capillary" box is checked.
Id: 3649	Title: Component: Area: Description:	1200 "save as active method" circumvents method security 1200 System Control - General If you have a method password to prevent anyone from editing or changing your method, the 1200's scan window option can circumvent this. If you change the MS scan parameters, then click the button "Save as Active Method" from within the 1200 module, it will write those changes to the method without having you enter a password.
Id: 3654	Title: Component: Area: Description:	System does not exit "clean" 1200 Installation/Configuration When making changes to the system configuration under "options" in the 1200 the 1200 module needs to shut down to make changes active. In the past this would mean rebooting system control. Now the 1200 exits and immediately when the 1200 screen is gone another 1200 screen appears totally mis-sized and reboots the 1200. The only way to get out of this badly sized 1200 module is to exit system control manually and restart system control. You have to do this otherwise the complete lower section including the output line and control line are not visible.
Id: 3663	Title: Component: Area: Description:	New Lens 1 setting (pulse) 1200 Installation/Configuration The new lens 1 setting in configuration is not saved the same way as the other settings (meaning after applying the change, the 1200 software would need to be restarted).
Id: 3734	Title: Component: Area: Description:	Vent cycle does not set temp back 1200 System Control - General When using the cool down and vent option the temperature for the ion source and transferline are set to zero. After pumping down the system again the temperature for the ion source is set back (to the set point) but it leaves the transfer line cold. It should put both temperatures back

Id: 3747	Title:	Coarse tune resets optimum detector
	Component:	1200
	Area:	System Control - General
	Description:	Every time that the Coarse Tune is run, it resets the "detector optimum" to 1000V. This invalidates the EDR calibration.

2000 MS Issues Resolved

Id: 3419	Title:	Filament should be turned off in bakeout (2000)
	Component:	2000
	Area:	ModWin - Temperatures
	Description:	Normally the filament, if on, is left on when leaving Manual Control. This is done to avoid switching the filament on and off more than is necessary. However, if a bakeout is being done then the filament will generally be on for hours. In this case it's worth turning it off. When the bakeout is complete the filament is turned on again before reentering Manual Control.
Id: 3686	Title:	2000: Transferline Bakeout Temperature Persistence & Preset Value
	Component:	2000
	Area:	ModWin – Temperatures
	Description:	The present preset Bakeout Temperature for Saturn Transferline is 170 °C. This is too low for significant bakeout/cleaning of typical column and assembly contaminates. Change the transfer line bakeout default to 220. Save the entered temperature.

4000 MS Issues Resolved

Id: 2287	Title:	Need adjustment parameter for high-mass calibration
	Component:	4000
	Area:	ModWin - Manual Control
	Description:	Users need to be able to enter the Expected and Observed high mass and have the mass calibration adjusted.
Id: 3208	Title:	4000: MRM and MSMS could be combined
	Component:	4000
	Area:	DAMeth - MSMS
	Description:	It would be easier for the user if the 4000 software only had a single MSMS function that changed from SRM to MRM if a second line was added to the method.
Id: 3223, 3226	Title:	4000: Use total cycle time in MSMS and AMD
	Component:	4000
	Area:	DAMeth - MSMS
	Description:	When using the MS/MS or AMD method type the scan time should be calculated based on the total time it takes to do all operations in the scan (not a single channel). The number of uScans is applied to each channel.
Id: 3557	Title:	Software crashes when leaving System Control
	Component:	4000
	Area:	System Control - General
	Description:	When closing System Control and the user allows the dialog box saying "Are you sure you want to close System Control" to time out, the dialog box will automatically reappear. Clicking "No" at this point and the screen is grayed out except for the tabs, and a chemis32.exe error is reported shortly afterwards.

Id: 3768	Title: Component: Area: Description:	Mass Cal Std Dev Error 4000 ModWin - General In the printout of the module attributes, the standard deviation is shown as 0.00 when it should be about 0.06.
Id: 3789	Title: Component: Area: Description:	4000: Autotune options preselected 4000 ModWin - Auto Tune Since the normal user in autotune selects all of the functions to do everytime it would be simpler if the autotune functions were preselected.
Id: 3839	Title: Component: Area: Description:	Upon communication error, upload and save Controller RAM 4000 ModWin - General When a communication error (or possibly some other failure) occurs, there is often the need to obtain detailed information than what is currently saved in the PSTSnn.BIN file). The Workstation has been modified to save additional information the next time it is started after a failure. It will generate several PSTS*. files, which could be sent to technical support in the event of a communications failure.

MS Data Handling Issues Resolved

Id: 3214	Title: Component: Area: Description:	Peak >peak size reject can be rejected MS Workstation Platform Quan MS - Cmpd Integration Under certain conditions during chromatogram processing, a Duplicate peak can be eliminated from the results when it should not be, even though its peak size is greater than the Peak Size Reject setting in the Integration Parameters.
Id: 3279	Title: Component: Area: Description:	Valley and Tangent Apex events on same point confuse results MS Workstation Platform Quan MS - Cmpd Quantitation Description: The area of small tangent peaks sometime can be reported for the main peak that they are on. This happens when the tangent peak apex event is on the same point as the tangent start. Processing should discard peaks whose start and apex events are on the same point.
Id: 3383	Title: Component: Area: Description:	Closing Automation file does not remove it from application workspace MS Workstation Platform Other When working with an automation file in the Automation File editor, closing the file does not remove the file from the workspace, so that trying to reopen the file (or open it in another applicaton) is prevented until the AFE application itself is closed.
Id: 3591, 3592	Title: Component: Area: Description:	Actual 1200 Method is Not Displayed for Data File MS Workstation Platform MSDataRev - Reports, View&Print In the 1200, only the Run Log is currently available in the Data File Information Dialog (available when clicking on the Segment Bar in MS Data Review) or Standard MS Reports. Though the Run Log includes (most, if not all of) the conditions as they were during the run, a display of the actual method that was executed should be available as well.
Id: 3624	Title: Component: Area:	Automation/Data Handling errors cause huge Sample Reports MS Workstation Platform Quan MS - General

	Description:	If problems in automation cause ms quantitation on a data file to fail, or if quantitation doesn't add a Results section to the file because it fails or there aren't any results, the printed Sample Report uses the default report method settings. This causes the Run Log to be printed for each file that fails, which can be tens of pages long.
Id: 3667	Title: Component: Area: Description:	Relative RT doesn't report correctly MS Workstation Platform DHMeth MS - Compound Table The rel RT peak itself gets reported correctly with a value of 1.00, but the other peaks all get reported as 'none'.
Id: 3132	Title: Component: Area: Description:	Sample List Editor doesn't handle write protected files correctly Other Component Other Open a write-protected sample list in the Automation Files Editor, make changes, close the editor, accepting the Save. Reload the file and observe that all your changes are GONE!
Id: 3806	Title: Component: Area: Description:	MSDR Integrate Plot doesn't use data file method MS Workstation Platform MSDataRev - General When Integrate Active/All Plot(s) is selected in the Plots view, the integration parameters that were last saved in the Integration Results dialog are used. If the data file has been quantitated the GlobalParams integration parameters from the data file should be used.
Id: 3909	Title: Component: Area: Description:	Print to PDF only does first 20 pages MS Workstation Platform MSDataRev - General Print reports are broken up into 20-page blocks in order to prevent them from hogging the printer and preventing other print jobs from being printed. This causes 2 problems: 1. People don't like parts of different print jobs to be interleaved. It's very confusing when different people/instruments are using the same printer. 2. When the printing is going to a PDF or a text file, it can result in multiple files that have to be pieced back together by the user, or sometimes nothing after the first 20 pages goes to a file..

Core Workstation Issues Resolved

Id: 3344	Title: Component: Area: Description:	Editing SampleLists can cause Autolink buttons to scramble AutoSampler Module System Control - Automation Build a SampleList that includes few Activate Method or Autolink calls in the Sample Type. Also fill in the AutoLink cells for all your calls. So far the spreadsheet should look right. Now edit the table using Delete and Insert. After doing that few times you will notice that the files listed in the AutoLink buttons do not line-up with the Activate Method or Autolink calls in the Sample Type. They are scrambled. The cells are actually having the correct info, but the buttons are not labeled correctly. Refreshing the window does not solve the problem. Also the Notes column has the same problem.
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Id: 3598	Title: CPAL Run File Error Log Feature Component: AutoSampler Module Area: Other Description: Add CPAL barcode errors associated with unreadable barcodes and barcode mismatches w/r to sample names, to the run file Error Log.
Id: 3619	Title: CPAL: Driver improperly handles incorrect injector position. Component: AutoSampler Module Area: Other Description: The driver is already aware that the requested injector does not exist, but... If the injector position is improperly stored, an error will occur and no injection will take place, but the driver will start the modules anyway... There are at least 2 situations to consider: (1) The incorrect position is accessible, but "in the air", so the PAL will not sense a physical injector, and will cause an error 115 'Vial Not Found'. (2) The incorrect position is not accessible, because other HW is in the way. This will cause an error 147, "Collision Error" The driver should sense such errors, know it did not inject, and not start the other modules.
Id: 3627	Title: CPAL: Enhanced Automix AspirateFrom Command Component: AutoSampler Module Area: Other Description: CPAL: Enhance the AspirateFrom automix command to include a user-specified air gap.
Id: 3628	Title: CPAL: Detection of Missing Tray Component: AutoSampler Module Area: Other Description: Add missing tray detection to errors that stop a run.
Id: 2552	Title: Sample list not closed from System control properly Component: Core Workstation Platform Area: System Control - General Description: A sample list did not seem to close properly in System control. Automation File Editor could not open the sample list as it was still "in use" by system control. The sample list had been closed (and was no longer visible on screen or under the windows menu) while a run was going, started from "inject single sample".
Id: 3075	Title: ShowMLG: Ability to copy and paste Message log entries Component: Core Workstation Platform Area: Other Description: When viewing the message log in ShowMLG there is no way to export that data to an electronic form (ie cut/paste). The only way to get a copy is to print (and not everyone has pdf printers yet). It should work like regular copy and paste (using <Ctrl-x,c,v as the shortcuts). Resolution: Ctrl+c or Ctrl+Ins copies the selected line to the clipboard. It can then be pasted in another application.

Id: 3076	Title: Component: Area: Description:	Cut, Copy, Paste, and Undo using current windows default shortcuts Core Workstation Platform System Control - General Cut, Copy, Paste, and Undo should work using the current windows default shortcuts of <ctrl-x, c,v, and Z> and should be displayed in the SW as doing so. The old DOS series of <shift-ins>, <shift-del>, and <control-del>, or whatever they are, should not be the displayed shortcuts. They can function, but should be the secondary level in the software.
Id: 3082	Title: Component: Area: Description:	Print Summary not available in 2 SampleLists Core Workstation Platform System Control - General The "Print Summary" is not available in the drop-down selection for the PS-400 and PS-420 SampleLists for MSWS systems.
Id: 3126	Title: Component: Area: Description: Resolution:	Software Should Recognize GC in Standby Mode Core Workstation Platform System Control - Automation The 3800 has a Standby Mode that sets the column temperature to a standby value if the GC is not run for more than a specified time period. This mode is terminated by reactivating the method. The problem is that when starting automation, System Control waits for all modules to be ready before activating the method, and the GC never gets out of standby mode. The 3800 method is reactivated at automation start if the GC is equilibrating.
Id: 3164	Title: Component: Area: Description:	Audit Control manual does not load even if specified so Core Workstation Platform WS Security Admin (21CFR11) Please assure that the audit control software manual is loaded when someone has the SN for this option and specified to load the manual. Currently it is not happening.
Id: 3190	Title: Component: Area: Description:	Have access to injection notes while editing recalc notes Core Workstation Platform System Control - Automation We want to see the injection notes in the recalc list. The simplest approach would be to display the Injection Notes in the dialog editing the Recalc Notes. The injection notes would be displayed in a read-only window from which text could be copied.
Id: 3404	Title: Component: Area: Description:	Message Log can get too big and cause havoc Core Workstation Platform System Control - Automation In the past, when the message log had a fixed name for each instrument, we ran into situations where it could get to big and crash system control. This is less likely to occur now, as we create a new log each time we start system control, and at each automation start, but for "process" applications where people use an infinite loop, it is still possible to reach message log sizes that would cause problems. Resolution: A new messagelog is created at a safe point during automation when the current log size exceeds a set value (1 Megabyte).

Id: 3427	Title: Component: Area: Description:	AutoLink command line should be quoted if needed Core Workstation Platform System Control - Automation Autolink commands including spaces in the file names fail. Adding quotes to commands that need it fixed the problem.
Id: 3535	Title: Component: Area: Description:	System Control - Sample List can stay dirty if injecting single samples Core Workstation Platform System Control - Automation If you open a Sample List in System Control, the file will be marked with a dirty flag so that it is not accessed while used by SC. If you close the file, the dirty flag will properly be removed. However, if you inject a single sample, then close the sample list, the sample list will remain dirty.
Id: 3572	Title: Component: Area: Description:	"Do you want to close System Control?" message default Core Workstation Platform System Control - General For V6.5, turn this message on by default.
Id: 3577	Title: Component: Area: Description: Resolution:	Windows cannot find Chemis32 help file Core Workstation Platform System Control - General If within an application you browse for data, you may not be able to find the on-line help later in the session. The help function was modified to always look for help files in the proper folder.
Id: 3673	Title: Component: Area: Description:	SMPEDIT: Closing file leaves title set Core Workstation Platform Chrom Applications After a file of any type is closed, its name is left in the caption of the application.
Id: 3834	Title: Component: Area: Description: Resolution:	Cannot preset method Core Workstation Platform System Control - General If the active method's directory is renamed/removed, then system control will not start up correctly. A default method file is re-created in the WS directory.
Id: 3364	Title: Component: Area: Description:	Documentation of 3800 PFPD AutoGain feature GC Module Other The on-line help does not describe the operation of the 3800 PFPD Autogain feature.
Id: 3647	Title: Component: Area: Description:	335: Displaying Chromatogram only does not work well LC Module ModWin - General When you select the Chromatogram only option in the 335 Status window the CDF will display the chromatogram and part of the Spectrum panel. Spectrum only option works fine.
Id: 2551	Title: Component: Area: Description:	Improve Navigation of Message Logs and System Logs Other Component Other For new message logs, added info about next/previous log, and navigation buttons to Log Viewer application.

Id: 3132	Title: Component: Area: Description:	Sample List Editor oblivious to write failure Other Component Other Improved handling of write-protected automation files
Id: 3595	Title: Component: Area: Description: Resolution:	Improvements to CAPSULE Advanced Application Other Component Other CAPSULE is an advanced application designed to encapsulate processes that do not support the AutoLink protocol. By design, capsule terminates only when it detects that the application it launched has itself terminated. 1) It would be nice to have an option to tell capsule that it should exit immediately. 2) Capsule appends the name of a current WS file (run file, smp, rcl, seq, meth) to a command line, but there is no way to add parameters after the file name. This is an issue for some applications, like Standard Reports and Interactive Graphics, which can specify a channel on the command line, but AFTER the file name. We need a mechanism to specify further parameters when composing the capsule command. 1) If a "-x" argument is provided (capsule -x), or capsule.exe is renamed to "launch.exe", then capsule will not wait for the application to terminate. 2) parameters after the file name token are now taken into account by the invoked application.
Id: 3685	Title: Component: Area: Description:	8400 volume info missing from reports Other Component Other The volume information is missing from results reports for both .SMS and .RUN datafiles for an 8400 running on a 3800.