

Varian MS Workstation Version 6.9.3 Release/Update Notes

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Overview

These Release Notes are organized into two broad categories:

- Items of Interest to All Users of the Varian MS Workstation Version 6.9.3
- Items of Interest to Users Upgrading from MS Workstation Version 6.9.2

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

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

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

General Operational Considerations

SYSTEM REQUIREMENTS

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

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

INSTRUMENTS SUPPORTED

MSWS 6.9.3 supports the following Varian MS instruments:

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

MSWS 6.9.2 SP1 does NOT include drivers for the 430-GC, the 920-LC or the 940-LC models. Proper operation of 1200 and 1200L instruments is not validated for MS Workstation versions later than 6.9.1.

ANTI-VIRUS SOFTWARE

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

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

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

WINDOWS POWER SCHEMES AND COMMUNICATION FAILURES

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

WINDOWS AUTOMATIC UPDATES AND COMMUNICATION FAILURES

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

USE OF MS ACCESS-BASED TEMPLATES

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

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

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

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

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

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

Installing the MS Workstation

BEFORE INSTALLING THE MSWS SOFTWARE

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

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

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

INSTALLING THE SOFTWARE

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

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

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

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

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

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

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

Update Ver 6.x to Ver 6.9.3 MSWS: Choose this option if a previous version of MSWS 6.x is installed. The serial numbers will be automatically re-entered. However, while the serial numbers for most 5.x options (EnviroPro, ToxPro, etc...) can be used with MSWS 6.9.3, serial numbers from pre-6.5 versions of the core MS Workstation software will not work with 6.9.3. You must purchase an upgrade to use the MSWS 6.9.3 software.

Install MSWS Software: Choose this option if no MSWS version is installed. You will need to provide a serial number for the MSWS and any of the options you purchased. Please review the terms of the licensing agreement. If you reject the agreement, the installation program will exit.

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

The Module Driver for the 1200, 1200L, 300-MS, 310-MS, 320-MS, and 325-MS is named "Quad Mass Spec" as it supports multiple models of quadrupole MS modules.

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

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

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

OPTIONS/SERIAL NUMBERS

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

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

MICROSOFT ACCESS

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

NIST MS SEARCH AND AMDIS PROGRAMS

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

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

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

MS Workstation Operational Considerations

MS WORKSTATION AND NETWORK OPERATION

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

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

MULTIPLE USERS ON A SINGLE MS WORKSTATION

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

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

CONCURRENT USE OF METHOD FILES

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

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

QUAD MS DRIVER

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

SATURN 2000 AND LC MODULES

If both the Saturn 2000 and LC Modules are selected for installation, then Saturn 2000 will be installed with data handling capability only. As the Saturn 2000 and certain LC Modules both use the same GPIB interface, their use is mutually exclusive.

MS DATA REVIEW

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

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

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

Known Issues in MSWS 6.9.3

450-GC

GC Status in Setup Ethernet Communications dialog

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

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

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

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

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

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

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

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

MS DATA HANDLING

When a transition is added to (or deleted from) an Acquisition Method Time Segment, it changes the physical channel for other transitions in the segment that are specified after it. For Quad instruments, the channel is changed for all transitions in the segment that have a higher Precursor mass. This will invalidate any existing compound table specifications in the data handling method that reference these transitions. A patch to fix this problem is available from Varian Technical Support for software versions 6.9.0 SP1 or later.

To fix the compound table when the patch is not installed, or if the acquisition method and the compound table are already inconsistent before the patch is installed:

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

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

NOTE: This patch will not fix the Compound Table if changes are made to the acquisition time segments (shortening a column or changing start time of segments). This issue will be addressed in a future release.

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

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

Items of Interest to Users Upgrading from MS Workstation 6.9.2

What's New in MSWS 6.9.3

The primary purpose of the MS Workstation 6.9.3 release is to provide support for the 325-MS and 460-LC Modules.

The 325-MS instrument is a more sensitive triple quadrupole instrument that contains a new API Interface (Vortex ESI or vESI). The 325-MS operates only in LC mode.

The 460-LC instrument is a new LC Autosampler that is a replacement for the Prostar 410, which will be discontinued in late 2009.

MS Workstation 6.9.3 contains all the HotFixes, Corrections, and Enhancements that have been released since the MS Workstation 6.9.2 release.

What's New in MSWS 6.9.2 SP1

The primary purpose of the MS Workstation 6.9.2 SP1 release is to provide support of the 225-MS Module (Integrated Pumping Solution version of the 200-MS Ion Trap).

The 450-GC Module now also supports the 2.03 version of 450-GC Firmware. Customers upgrading to 6.9.2 SP1 who have a 450-GC Firmware version prior to 2.03 will need to upgrade the 450-GC Firmware to Version 2.03.

In addition, a SIS option key is no longer needed to run SIS methods on the 2000/200-MS systems. Users who do not have the option key can run SIS methods by upgrading to 6.9.2 SP1.

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

HotFixes included in 6.9.3

None

HotFixes included in 6.9.2 SP1

Id: HF 100033	Title: Proper Indexing of Manuals Area: Documentation Descr.: The Index and Table of Contents was corrected to fix the inability of some files that were not correctly linked.
Id: HF 100034	Title: Manual Integration Crash of MSDR Area: MSDR – Manual Integration Descr.: This is a correction for Manual Integration Crash that has been observed when performing manual integration on a large number of compounds in MSDR.
Id: HF 100036	Title: Correction for Leakage Current Area: Quad - System Descr.: Whenever the filament is turned on, readings of filament leakage are collected and an average value is computed. This average value is added to the filament current that has been set by the user. Previous versions did not correct for the leakage current.
Id: HF 100037	Title: Ready State Module Correction for 450-GC Area: 450-GC – Method Download Descr.: This problem has been observed when multiple methods are activated in a sample list and starting temperatures were different. The injection would occur before the GC reached the setpoint for the currently loaded method if it was different from the last method used in the sample list. The Ready State has been changed so that the 450-GC driver does not go Ready until the temperature setpoint for the method just loaded has been reached.

Core Workstation Platform

CORRECTIONS IN MSWS 6.9.2 SP1

Id: 6858	Title: ACS Editor failure to load sets after method conversion Area: Active Compound Set Editor Descr.: In previous versions, a compound set could not be loaded after method conversion. In this release, the method converter now clones the ACS sets properly, so that the sets defined in the old method work correctly with the converted method.
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200-MS & 2000 GC/MS Ion Trap Module Changes

GENERAL INFORMATION NEW IN 6.9.2 SP1

Support for the new 225-MS Module was included in 6.9.2 SP1.

A SIS option key is no longer needed to run SIS methods on the 2000/200-MS systems. Users who do not have the option key can run SIS methods by upgrading to 6.9.2 SP1.

240-MS/4000-MS Ion Trap Module Changes

CORRECTIONS IN MSWS 6.9.2 SP1

Id: 6861	Title: Increase of Getter Cut-Off Temperature Limit Area: 240/4000-MS Descr.: Some getters can operate at higher temperatures than the previous temperature limit of 475 °C. The temperature limit has been increased to 510 °C.
Id: 6892	Title: Reduce False Positives in Quick Verify Emission Leakage Test (Internal) Area: 240/4000-MS Descr.: After the end of each acquisition, the Emission Leakage test is performed, but the filament leakage may not decay enough so that the test fails. In addition, turning the heaters on or off can cause a perturbation in the filament current reading causing a failure. In order to reduce the number of false positives during the Quick Verify Emission Leakage test, the following changes have been made: 1) The tolerance has been increased from 5 to 8 µA 2) At the end of each acquisition, the test will be repeated three times with a delay of 30 msec if the initial test fails. The delay and number of repetitions will add enough time for the leakage current to decay. Also, repeating the test four times will ensure that there will be at least one test where none of the heaters are being turned on or off.

500 LC/MS Ion Trap Module Changes

ENHANCEMENTS IN MSWS 6.9.2 SP1

Roughing Pumps Types identified

In the Startup/Shutdown and Diagnostics Screens, the type of the roughing pump is now identified (HS652 or MS40+). Previously, the pumps were identified as only Roughing Pump 1 and Roughing Pump 2.

CORRECTIONS IN MSWS 6.9.3

Id: 6132	Title: Precursor High Mass not stored and Precursor Low Mass is scaled incorrectly Area: 500-MS - Data Descr.: The display of the Precursor High Mass and Precursor Low Mass in the Summary Information View of the spectrum of MS/MS has been corrected.
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MS Data Handling Changes

ENHANCEMENTS IN MSWS 6.9.2 SP1

Id: 6875	Title: Improve spectra background correction in quantitation Area: MS Data Review – Review Results Descr.: Background correction points are no longer constrained to the compound Integration Window during quantitation. All points within a window of +/- (50 x number of points/sec) will be considered. To eliminate distortion by co-eluting peaks, background correction points that are on a peak are excluded.
Id: D-01836	Title: Improve spectra background correction in Plots View Area: MS Data Review – Plots View Descr.: Previously, when a spectrum was selected that is outside of the background correction points in a chromatogram, background correction used a straight-line extrapolation based on the two nearest background correction points. Now, the nearest background correction point is used directly.

CORRECTIONS IN MSWS 6.9.3

Id: 6900	Title: Corruption of 5.x files when cancel conversion to 6.x files Area: MS Data Review – General Descr.: Canceling the conversion of a 5.x datafile would corrupt the datafile so that it is no longer able to be used in 5.x versions of the software. A fix has been implemented where the datafile will be automatically converted to a 6.x datafile, but the user will have the option to save the datafile in the old file format so that it can be used in 5.x versions of the software.
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Id: 6898	Title: Exporting to ASCII does not shift cells correctly when point excluded from curve Area: MS Data Review – Reports and Printing Descr.: When exporting a Calibration Block Report to ASCII with excluded Calibration Curve Points, the columns were not shifted correctly in previous versions of the software. This problem has been fixed in the 6.9.3 release.
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CORRECTIONS IN MSWS 6.9.2 SP1

Id: B-04466	Title: PP Click-and-Drag noise sometimes wrong Area: MS Data Review – Plots View Descr.: When Peak-to-Peak noise was calculated for a manually-selected region in a chromatogram, the Drift Corrected value could be calculated incorrectly if the baseline was changing rapidly
Id: B-04400	Title: ASCII calibration block reports not updated Area: MS Data Review – Review Results Descr.: When calibration data are modified in the Results View, the modifications were included in the Calibration Block reports when they were printed, but not when they were exported to an ASCII file.

Quadrupole MS Module Changes (1200/1200L/300-MS/310-MS/320-MS/325-MS)

GENERAL INFORMATION NEW IN 6.9.3

The MS Workstation 6.9.3 release is focused on the control of the new 325-MS LC/MS instrument.

Roughing Pumps Types identified

In the Pump Statistics Screen, the type of the roughing pump is now identified (HS652 or MS40+). Previously, the pumps were identified as only Roughing Pump 1 and Roughing Pump 2.

CAS and Compound Name Fields in Scan Table

It is now possible for users to add CAS and Compound Names to the Scan Table in both the Method Editor and System Control.

Autotune Changes

In LC systems (3x0), if the starting temperatures and pressures are not the recommended at the beginning of Autotune, the user will be prompted to change these values. If Cancel is clicked, the Autotune will stop. If the user clicks ok, a new dialog will appear so that the user can enter an appropriate tuning value. In this new dialog, the user can enter a new value or use the default and click ok. The Autotune will continue after the new temperatures and pressures are reached. If the user

clicks cancel, the Autotune will proceed with the “not recommended” value and an error will be logged in the Tune Report.

CORRECTIONS IN MSWS 6.9.2 SP1

Id: 6862	Title: Transferline Heater may remain on after System Control is closed Area: 3X0-MS - System Control (GC) Descr.: A correction was made to ensure that the Transferline Heater does not continue to heat at 100% duty cycle after System Control is closed. If System Control is closed, it will set the temperature to 0 to turn off heaters. When System Control is reopened, it will use the last temperature setpoint used before the shut down.
Id: 6872	Title: Aborting Single Sample Run causes Quad to Hang Area: 3X0-MS - Acquisition (LC) Descr.: If a single sample acquisition was aborted and another run started, the Quad Module would hang if the 212-LC was in the Auto-Start box. This has been corrected in the current release.

431-GC Module Changes

CORRECTIONS IN MSWS 6.9.3

Id: 6867	Title: Lose column flow parameters if you turn on pressure pulse Area: GC Module – Method Editor Descr.: Turning on a Pressure Pulse after changing the column flow parameters within the 431-GC Method Editor will no longer effect the previously changed column flow rate.
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