MassLynx 4.2 SCN 1024 Release Notes

General information

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Contacting Waters

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www.waters.com	The Waters website includes contact information for Waters locations worldwide.
iRequest	Request technical support for your Waters instruments and software. iRequest is a free and secure Web service that allows you to obtain quick answers from our online Knowledge Base, request support and service for Waters instruments and software, or schedule a planned service activity. **Note:** In areas managed by authorized distributors, iRequest may not be available. Contact your local distributor for more information.
Telephone and fax	From the USA or Canada, phone 800-252-4752 or fax 508-872-1990. For other locations worldwide, phone and fax numbers appear in the Waters Local Offices information.
Conventional mail	Waters Corporation Global Support Services 34 Maple Street Milford, MA 01757 USA

Updated information

Refer to the Waters website (www.waters.com) and click **Support** > **Support Documents and Downloads** for updates to this document.

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MassLynx Software Change Note 1024

Introduction

MassLynx Software Change Note (SCN) 1024 is for MassLynx version 4.2. It supersedes the various SCNs described below. SCN 1024 includes new enhancements, fault fixes, and concessions as described in the Enhancements, Fault Fixes, and Concessions sections of this document.

Superseded SCNs

MS	Superseded SCN Version
Xevo TQ-S micro	SCN 1019
Xevo TQ-S cronos	SCN 1019
Xevo TQ-XS	SCN 1012
Xevo TQD	SCN 985

Supported drivers and EPCs

MS	Supported EPCs
Xevo TQ-S micro	• The original Kontron EPC (700010270) • The new variant of Kontron EPC (700011091)
Xevo TQ-S cronos	• The new variant of Kontron EPC (700011091)
Xevo TQ-XS	• The original and new variant of Adlink EPC (700011219)
Xevo TQD	• The original Adlink EPC (700005817) • The new variant of Adlink EPC (700011089)

LC/Inlets	ICS Version
GC - Agilent 8890	• Waters Support Layer Version 3.3.0.14 • Agilent GC Driver Version 2.6 Update 3
CTC PAL3 RSI	RC .NET Version 1.4.0.16

Supported components

MassLynx 4.2 SCN 1024 was tested with **Waters Driver Pack 2021 Release 1**. It is possible that other versions of driver packs work with this SCN. For details, contact your local Waters specialist.

The MassLynx version 4.2 SCN 1024 installation supports the following components. For configuration recommendations, contact your local Waters specialist.

Inlet Components
ACQUITY UPLC, H-Class, I-Class, and M-Class Systems
ACQUITY Binary Solvent Manager
ACQUITY Sample Manager
ACQUITY FLR Detector
ACQUITY Sample Organizer and CPSO
ACQUITY Column Manager
ACQUITY PDA Detector
ACQUITY TUV Detector
ACQUITY ELS Detector
ACQUITY FLR Detector
ACQUITY Open Architecture System (Waters 2777 Autosampler)
ACQUITY Isocratic Solvent Manager
ACQUITY Sample Manager-FTN
ACQUITY Quaternary Solvent Manager
ACQUITY µBinary Solvent Manager
ACQUITY µBinary Sample Manager-FL
ACQUITY Sample Organizer
Waters Pump Control
Waters 2545 Pump
Waters 2996 PDA

Inlet Components
Waters 2695 (controlled via GPIB)
eAlliance (controlled via GPIB)
Agilent 8890 GC
CTC PAL3 RSI (with Agilent GC 8890 only)
ACQUITY Arc
Waters 2777C Autosampler
eSAT/IN detector
nanoACQUITY

Operating system

MassLynx 4.2 SCN 1024 is supported on the English versions of Microsoft Windows 10 Enterprise LTSB 1607 on a Waters-supplied acquisition workstation.

Security

MassLynx 4.2 SCN 1024 supports both basic and full MassLynx Security configurations.

SCN 1024 installation procedure

MassLynx 4.2 SCN 1024 is a complete installation of MassLynx 4.2.

Notes:

- This procedure requires Windows administrator privileges, and the user must log on to the computer as a local administrator (not any other/domain user with local administrator rights).

- Do not attempt to modify or repair an installation. Modifying or repairing an installation is not supported.

Preparing for installation

Before installing MassLynx 4.2 SCN 1024, remove any existing MassLynx or MassLynx SCN installations using the **Programs and Features** utility in the Windows Control Panel.

To remove existing software applications:

1. Close any open software applications.

2. Save and back up all application manager files residing in the MassLynx directory, such as method files, test tables, and report scheme settings.

   Note: Files in the MassLynx folder may be removed from the PC when you uninstall MassLynx.

3. Open the Windows Control Panel, select the **Programs and Features** utility, and determine whether the following applications are installed. If they are, uninstall them using the **Add/Remove Programs** feature.

   - MassLynx stand-alone applications

   - ACQUITY components

   - Instrument drivers, such as Waters Pump Control, Waters 2777C drivers, or Agilent drivers

   Note: Use the Deployment Manager to remove the Waters Pump Control, if necessary.

4. If you uninstalled MassLynx, restart the computer.

5. After you uninstall MassLynx applications, determine whether the *C:\Program Files (x86)\Micromass Utilities\ICOP* folder remains on the computer. If it does, delete it.

Installing MassLynx 4.2 SCN 1024

To install MassLynx version 4.2 SCN 1024:

1. Insert the MassLynx SCN 1024 installation media into the appropriate drive.

2. Open Windows File Explorer and browse to the folder where the installation media is present. Right-click *Setup.exe* and select **Run as administrator**. Close File Explorer and any other open windows, apart from the MassLynx installer window.

3. Follow the installation prompts.

4. Click **Finish** to complete the installation.

5. Restart the computer and log in to Windows.

6. Restart the instrument embedded PC.

ACQUITY console for MS-only system configuration

Note: Skip this section if you plan to configure ACQUITY inlets.

To install the Local Console Controller:

1. Start MassLynx and open the **Inlet Editor**.

2. Select **Tools** > **Instrument Configuration**.

3. In the Deployment Manager, click **Setup Instruments**, and then install **Local Console Controller**.

4. Restart the computer.

Installing inlet system drivers

To install inlet system drivers:

1. Insert the driver pack installation media that came with your LC system.
2. Run *Setup.exe* to start the Deployment Manager, click **Setup Instruments**, and then select a custom install. Ensure that you select the instruments required for your configuration.
3. Follow the wizard prompts and complete the installation process.
4. Restart the computer before continuing the inlet system configuration.
5. Start MassLynx and open the **Inlet Editor**.
6. Select **Tools** > **Instrument Configuration**.
7. Click **Configure** to launch the Inlet Configuration dialog box and complete the configuration of the inlet system.

Installing drivers for Agilent GC 8890 and CTC PAL3

To install drivers for Agilent GC 8890 and CTC PAL3:

1. Insert the MassLynx 4.2 SCN 1024 installation media and open the folder in the installation media.
2. Open the **ICF V3.3.0.14** folder, click **Setup**, and follow the instructions within the installation wizard. Choose Typical installation when prompted.
3. In the ICF V3.3.0.14 folder, open the PAL3 RC.Net Driver V1.4.0.16 folder, and then double-click to run the install package.

Configuring Agilent GC 8890 and CTC PAL3

Agilent 8890 GC Firmware version 2.0.0.291 was validated with this SCN. This is the minimum version required for support of the Agilent 8890 GC with MassLynx.

To configure Agilent GC 8890 and CTC PAL3:

1. Communication with the instrument through Ethernet is established by connecting one cable from the CTC PAL3, a second cable from the MS instrument (MSD), and a third cable from the GC to an Ethernet hub. The hub connects to the PC via another Ethernet cable. The PAL3 I/O cable connects to the GC by contact closure.
2. From the GC, the Event cable connects to Event 1 on the Mass spectrometer.

Configuration prerequisites

1. Launch the Control Panel from the Windows Start menu.
2. Double-click on the **Network Connections** application.
3. In the **Network Settings** window, right-click on the Ethernet device connected to the instrument and select the **Properties** option.

4. In the LAN properties dialog box, select **Internet Protocol (TCP/IPV4)** and click **Properties**.

5. In the **Internet Protocol (TCP/IPV4) Properties** dialog box, ensure that the IP address and subnet mask are set as follows:

   - Select **Use the following IP address**.

   - Set the IP Address to: `192.168.000.xxx.` (This value must be different from the IP address of the GC/CTC PAL3 instruments).

   - Set the subnet mask to: `255.255.255.000.`

6. Click **OK** to close the **Internet Protocol (TCP/IPV4) Properties** dialog box.

7. In the **LAN Properties** window, click **OK** to complete the LAN configuration setup.

Configuring PDF printing

In order for MassLynx to print to PDF format, a suitable print driver must be installed.

The TargetLynx XS report option to print to PDF requires that there be a print driver named "Adobe PDF". A PDF print driver can be renamed using Windows Printer Properties if required.

To enable PDF support for OpenLynx, there must be a print driver named "Adobe PDF" and it should be configured to automatically (without user prompting) output PDF files to the configured open access report folder (normally *C:\MassLynx\OALogin\ReportDB*).

Installing stand-alone applications

Note: This instruction is for the installation of OALogin, OAToolkit, Diversity (OpenLynx) Browser, and TargetLynx XS Browser if you have not installed MassLynx software.

If any of these applications are already installed, you must remove them, by using the Windows **Programs and Features** utility in the Windows Control Panel, before installing the SCN 1024 version.

To install a stand-alone application:

1. Close any open software applications.

2. Insert the MassLynx SCN 1024 installation media.

3. Navigate to the Applications folder on the installation media and select the folder for the application required.

4. Run *setup.exe*.

5. Follow the instructions within the Installation Wizard.

6. Click **Finish** to complete the installation of the SCN 1024 files.

Uninstalling MassLynx

To uninstall MassLynx:

1. Close MassLynx and any open software applications.
2. Restart the computer.
3. Uninstall MassLynx using the **Programs and Features** utility in the Windows Control Panel.
4. Uninstall all ACQUITY and other drivers that you have installed.
5. Restart the computer.

MS

Enhancements

The following table lists the software enhancements included in SCN 1024.

General
Two additional menu items are added to the main MassLynx window - **Help** menu. You can use these menu items to open and navigate the **Waters Support** page and the **Waters iRequest** page on the Waters website.
Some of the column names in the sample list "Customize Field Display" pane did not display the complete text. The dialog size has been increased to display the full column name.
Acquiring data in full security is now much faster, especially when acquiring multi-function data over a network to a shared folder.

Fault fixes

The following table lists the software problems fixed in SCN 1024.

Fixes
At the start of a sample run, the linked calibration file did not load correctly when the samples were submitted from different projects or with different tune files. This issue has been fixed.
When creating a new project, sometimes the warning dialog for importing the project would appear. This issue has been fixed.

Concessions

The following tables list the known software issues and workarounds for SCN 1024.

General concessions

General
A sample list batch cannot be modified after it has been submitted. If you need to modify the batch, stop and update, and then resubmit the batch. If you are using **Load Ahead**, ensure to purge the pre-aspirated sample prior to restarting a batch.
Accessing MassLynx from an unsupported PC via Microsoft Windows Remote Desktop may cause problems with MassLynx, including unresponsiveness or halting of acquisitions. This is more likely to occur when using a touchscreen or touchpad.
Desktop-only install – an incorrect error message stating "Failed to create new project" may appear when creating a new project. You can safely ignore the message. The project will be created as required.
Initial Conditions Method Events Reservoir Selection does not switch reservoirs correctly. Instead, you should use a timed method event.
MassLynx may become unresponsive if a user selects **Network** from the **Print Setup** dialog box. Configure printers in the operating system first. They will then be available in MassLynx **Print Setup** without the need to click **Network**.
Selecting the "USB" option in the Camera Application settings with defaults will no longer display an image. **Note:** The Camera application can be accessed via the Tune page. The following settings are required to give an image: • Video Norm: Pal_B • Video Format: Y800 (768x576) • Frame Rate: 25 • Input Channel: 00 • Video: Composite
The shutdown task options **Source Gas On** and **Source Gas Off** are available only after toggling the Ion Mode or starting an acquisition every time MassLynx is started.
When requesting a scanning experiment that is outside of the calibrated mass range, you must choose whether or not to apply the calibration. If you choose not to apply the calibration, the loaded calibration details will still be stored in the Experimental Record even though the calibration wasn't applied.
When switching MassLynx projects, the sample list browser may occasionally open in an incorrect project. If this occurs, browse to the required project.
When using nanoACQUITY, after you force a run to stop, your access to control the flow and composition may be locked on the **Additional Status** page. If this occurs, reset communication in the Inlet Editor (select **LC** > **Reset Communications**).

Tune page concessions

Tune Page
After switching Ion Mode, the tune page can occasionally appear unavailable (greyed out). Reselecting the required Ion Mode or navigating away from the tune page will correct this issue.
In Full Security, switching between users with different Ion Mode selections does not instigate automatic Ion Mode change detection. Always check and switch to the correct source type for the user.
When using an ASAP source, the Ion Mode selection may become unavailable. Use the console to swap Ion Modes, or physically change the source.
Occasionally, when changing Ion Mode, the instrument does not switch to the correct polarity. To correct this issue, reinitialize the instrument.
If a single-channel SIR function is used in a multi-function experiment, the first scan of the SIR will be repeated once before the rest of the experiment cycle commences.
If changing the source while in operation, it is recommended that the instrument be switched into Standby and back to Operate when the new source is fitted to ensure the source ID updates.
On some occasions, in APGC source mode, the tune page may no longer control the auxiliary gas value. If this happens, the corresponding readback may not show the correct value. Solution: 1. Put the instrument into Operate mode.   2. Close the tune page, open Windows File Explorer, and navigate to the *C:\MassLynx* folder.   3. Open the tune page and switch on API gas. The auxiliary gas can be controlled again.

Console/IntelliStart concessions

Console/IntelliStart
The console needs to finish loading before you select any options. Closing the console before this point can cause it to enter an error state.
When opening the console for the first time, the console plots sometimes do not appear. Close and reopen the console to display the plots as expected.
When using NanoFlow in IntelliStart, the manual optimization plotting graphs may be blank if you open the page while the source temperature is settling. Closing and reopening the console will return the plots to normal.
When using NanoFlow and a single syringe pump with IntelliStart, you must run the resolution and calibration stages independently to obtain separate resolution and calibration reference files.
The file name in the Sample Tune Develop Method can sometimes fail to populate the file path correctly. This happens when the Start button is clicked to launch the "Sample Tune Develop

Console/IntelliStart

Method (STDM)" window, and then a different tune file is opened in the tune page, and then you return to the STDM tab, delete the existing file paths, and start typing. The workaround is to manually type the full path in each field.

If you close and reopen the console during an IntelliStart sequence, IntelliStart does not recognize the sequence or its results when it completes.

Manual Optimization occasionally fails to use the selected Sample Tune Method Develop IPR file. You can select the correct IPR file in the **Manual Optimization** window.

The Rear Panel pages inject start indicator does not update on contact closure. Event In1 is indicated via the Event In display, and Event In 2 is not shown.

If using IntelliStart with a NanoFlow source, you must ensure that a stable beam is present before starting the IntelliStart sequence.

When running a multiple-polarity Sample Tune Develop Method, the overall process returns as **passed** with a green check mark if one of the polarities successfully completed. In this scenario, a health check indicates which polarity failed to complete as expected.

On rare occasions, when doing an IntelliStart Resolution routine and **Print Report to PDF** is selected, the application may fail when trying to open the report. The resolution, however, is completed normally.

IntelliStart-created methods are not optimally sorted. You must open them in MS Method Editor and then save them.

Occasionally, when running IntelliStart calibration, the tune page may remain locked even after calibration passes with a green check mark. If this happens, click the **Stop** button in the ACQUITY Console, close MassLynx, restart the instrument, and run Calibration again.

The tune page readback does not match the setting when the Console Manual Optimization page is active. Tune page and Manual Optimization cannot control the instrument at the same time.

When using IntelliStart in secure mode, lock symbols on the IntelliStart main page indicate that additional user permissions are required to access certain features. The following permissions are defined as required:

● Required. ◆ Required depending upon actions	Tune Page – Enter tuning window	Tune Page - Enter System Console	Tune Page - Enter Autotune	Tune Page - Create tune file	Tune Page - Alter tune file	MS Calibration - Create new file on disk	MS Calibration - Alter existing file on disk	Acquisition - Start calibration acquisitions	MS Method - Create new file on disk	MS Method - Alter existing file on disk
Instrument Resolution	●	●	●	●	●					
Instrument Calibration	●	●	●			●	●	●		
Sample Tune	●	●	●	◆	◆					
Method Developer	●	●	●						◆	◆
System Check										
Manual Optimization	●	●			●					

MS Method Editor concessions

MS Method Editor

When creating an SIR function, the **Undo**, **Redo**, and **Clear All** buttons have no effect on the Auto Dwell entries.
When changing the default PICS parameters via the drop-down menu, you should open and save all MRM functions that contain PICS to ensure that the parameters are applied correctly.
Waters recommends that you do not use ScanWave MS. If you do, it is only valid to have more than one ScanWave function in a method if the start and end times of the ScanWave functions are the same or if they do not overlap. Non-ScanWave methods are not affected.
The following message may appear when you are creating methods: "The dwell times chosen result in a cycle time below the recommended 80 milliseconds for ion mode switching. Should the dwell times be automatically updated?" If you do not select automatic update of dwell times, a reduction in instrument lifetime could result.
When running with a security-enabled system, limit experiments to a maximum of 250 MRM or SIR functions (with up to 32 channels each). Execution of experimental methods with more than 32 functions results in a drop in system performance.
Method Event initial settings should be used for events that are to occur at the time 0.0. If the required event is not available in the initial settings, it should be set to the time of 0.01.

MS Method Editor
When using MassLynx to record PDA or TUV channel data, a maximum of 1023 functions should be used in the Method Editor.
When assigning the smoothing parameters in Phosphopeptide, setting maximum values in both "Peak width" and "No. of smooths" can occasionally cause the Tune page to lose communications with the Instrument. It is recommended that both are set to less than 50% of the maximum allowed value.
If you enable V-sorting on a method and then add a SIR/MRM function with multiple channels, it could show incorrect dwell times even though the method is correctly written to the disk. Closing the channel function windows and opening them again corrects the display issue.

Additional information

The following tables list additional information for SCN 1024.

General
All ESCi experiments should be run in ESCi Ion Mode, not ESI Ion Mode.
When you first connect to the NanoFlow source USB camera, a message appears requesting the location of the camera driver. Find the driver at *C:\Masslynx \USBCameraDriverForWindows7*.
MassLynx does not support the Windows "User switching" option. To switch desktop users, exit MassLynx, log off, and then log in as another user.
If you need to remove instruments from the inlet configuration via the inlet Configuration Wizard, it is recommended that you do not uninstall the instrument control software (ICS) for the unwanted instruments.
When MassLynx security is closed on a standalone PC, the tune page may sometimes hang. If this happens, it will not be possible to log in to the MassLynx Security Manager (MSM). You will be warned that some MassLynx applications are still running. If this happens, restart the computer before logging into the MSM.
Occasionally, Windows Firewall could turn on by itself due to a Windows update or an update by your IT department. If there are no communications with the instrument or if you notice Windows Firewall is enabled, you must close MassLynx, disable the Windows Firewall from the Windows Control Panel, and then start MassLynx again.
When setting up shutdown methods, MS shutdown actions should be placed after LC shutdown actions in MS error methods to ensure that LC actions are able to complete even if MS communication is not available. LC shutdown actions should be placed after MS shutdown actions in LC error methods to ensure that MS actions are able to complete even if LC communication is not available.
In dual-polarity experiments, the experiment report will show all "actual" readbacks in the polarity of the last active function.

Tune Page

If the mass differs significantly between one MRM/SIR trace and the next, and you are running with Manual Interscan delays, you might need a larger ICD/ISD.

With an ionKey source, to use a TriZaic tile, you should still select the ionKey source tab and alter the defaults as required for the TriZaic tile.

When the ASAP option is fitted to the API source, the shaft must be removed momentarily in order for the Source Recognition dialog to identify the probe.

Do not switch the instrument to Standby mode while running the Detector Gain Wizard. Ensure that you stop the wizard before switching the instrument to Standby mode.

After linking a calibration to a tune file on the tune page, the link is not permanently stored until you save the tune file.

When running a sample list for Xevo TQ-XS and TQ-S micro/cronos with 1024 functions (with or without PICs) or Xevo TQD with 512 functions, you must disable the "Use Spike Removal" option in the instrument settings. To do this, select Setup > Set Instrument Threshold, and clear the Use Spike Removal check box.

Console/IntelliStart

When using an ionKey source, IntelliStart functionality is supported only for Positive Ion Mode.

When using an ESCi source to perform an ES-only Sample Tune Develop Method, ensure that the APCI probe temperature matches the Desolvation temperature required. Set the APCI probe temperature via the APCI tune page.

To use the Waters 2777/Waters 2777C Autosampler with the IntelliStart LC/MS System Check in regulated Full Security mode, do the following:

1. Copy all files from *<MassLynx>\Default.PRO\ACQUDB\ to <MassLynx>\SystemQC.PRO \ACQUDB* and ensure that existing files in the destination directory are not overwritten.

2. In MassLynx, log in as a regulated user, select **Import Project**, and then choose the *SystemQC.PRO* folder (this generates checksums for the copied files). The LC/MS System Check now works as expected.

IntelliStart is not used in APGC mode. You need to perform calibration manually when in APGC mode, or use the ESI calibration if you just switched over.

In IntelliStart, the advanced setup resolution and calibration Mass Range selected must encompass at least four masses present in the selected reference file.

A manually created calibration file that is linked to a resolution file created via an IntelliStart analysis is not recognized by the IntelliStart system. When you reselect the analysis type via the console, IntelliStart continues to use the original linked calibration file.

It is advisable to compare your mass of interest with the calibration check previously performed, to ensure that the peak is not too close to the acceptance window. Also, if the beam check fails, confirm that the cone voltage has been applied correctly.

Console/IntelliStart

Do not schedule a LC/MS System Check to run when another LC/MS System Check will still be active.
Run a LC/MS System Check only after any previously submitted batch has been completed.
Ensure that vial inputs are correctly assigned before running a LC/MS System Check.
For the IntelliStart LC/MS System Check to complete for both positive and negative ionization modes, you must execute the individual analyses separately.
The two ISD checks "LC/MS System Check Has Not Been Performed" and "LC/MS System Check Failure" have a higher priority than many of the other IntelliStart checks. To see these other IntelliStart checks, clear the selections for the two higher priority checks via the **Configure > IntelliStart Configuration** menu.
If a LC is not present in the system, the ISD checks "LC/MS System Check Has Not Been Performed" and "LC/MS System Check Failure" should be disabled from the system.
Use Manual Optimization only after a successful Sample Tune Develop Method.
If a sample tune file that has been generated by IntelliStart is overwritten at any point, the error message "sample tune is invalid" appears.
Printing from the ACQUITY logs will print all entries; to print a single log, first print to PDF, and then select the relevant log.
Additional reference files are available in the folder *C:\MassLynx\Ref\Archive*. If any of these files are required, they must be copied to *C:\MassLynx\Ref*.
When setting up a LC/MS System Check to verify the retention time window and ensure that the height of the QC peak of interest is greater than 5% of any other peak in the Chromatogram, if no retention time window is selected in the LC/MS System Check run, all other checks will be based on the largest peak in the Chromatogram.
To stop a LC/MS System Check after it starts, go to the MassLynx sample list and press Stop, and then go to the inlet page and press the stop hand.
If you are running a LC/MS System Check in opposite polarity to the tune page, the experiment used should contain at least one function in the polarity of the tune page.
The experiment used to conduct a LC/MS System Check should not contain both scanning and static functions (i.e., only MRM/SIR or scanning, not mixed mode).
Smoothing is disabled by default in System Check.
Prior to running the IntelliStart calibration pre-check, check the signal intensity of masses of interest to ensure that the correct cone voltage is selected for the calibration compound in use.
Factory default resolution parameters will be loaded and checked during a resolution sequence that has a target resolution of less than 0.75 Da, unless specifically overridden for each run through the advanced options.
To avoid the calibration screen continually prompting for user input when printing to file, you must configure your PDF print driver options to let IntelliStart automatically produce PDFs in the IntelliStart.pro folder without requiring user input.

Console/IntelliStart

The IntelliStart Sample Tune Method Develop Combined infusion syringe flow rate is not automatically set according to the ACQUITY flow rate; it defaults to a value of 10 µL/min. This default may not produce a stable beam at high LC carrier flow rates.

When using the multiply charged function within the IntelliStart Sample Tune Develop Method, the mass to be entered is the mass to charge ratio (*m/z*) of the precursor charge state of interest. The multiply charged function will then complete the production scan to the mass range defined by the type of analysis under investigation. If the mass range is not sufficient to observe the required mass fragment, a new analysis type will be required with an appropriately calibrated mass range (up to the limit of 2048 *m/z*).

Entering the characters * / \ ? as part of names or file names causes an error. If the error is triggered, click **Continue** and rename the file using valid characters. Waters recommends using only the English alphanumeric, hyphen, and underscore characters.

When running a positive and negative Sample Tune Method Develop, only the most intense peaks are detected, not the most intense peaks in each polarity. To get the most intense peaks in each polarity, run the sequence in one Ion Mode and then the other mode, and append the results to the first existing method.

When running a calibration with the print option enabled, you must select the Print or Save option when the print dialog box appears. If you do not select Print or Save within a few minutes, the fluidics system can drain. The fluidics refill does not initiate automatically, because the software is waiting for a user response.

MS Method Editor

If an MS Method was created on a previous version of MassLynx, open the file in the Method Editor and re-save it before running it on the instrument. This ensures that the experiment's functions will run in the order shown in the Method Editor.

When setting up timed events that involve fluidics, ensure that you give scheduled events enough time for each operation to complete. When you attempt a fluidics timed event while a previous fluidics timed event is still in operation, the later event might not execute.

Enabling and disabling the MRM/SIR V-sort algorithm can take up to three minutes if the experiment contains a large number of functions.

When creating method events, there should be no events in between the solvent delay start event and the solvent delay end event.

Use short scan times for both the "Switch From" and "Switch To" functions when running Survey Functions. Using long scan times reduces performance when switching between functions.

INLETS

Enhancements

The following table lists the software enhancement included in SCN 1024. For enhancements and fault fixes related to ACQUITY inlets, see the release notes for the ACQUITY driver pack.

SCN 1024 supports ACQUITY Arc

Concessions

The following tables list the known software issues and workarounds for SCN 1024.

General
The eSAT/IN channel description is saved only when you click the "x" to close the Method Editor.
The Waters 2545 pump is shown as Waters 2535 in the experimental record.
Waters recommends that you use a scan rate no higher than 1 scan per second with the Waters 2996 detector.
When running an ACQUITY Open Architecture System, enable the column temperature data channel in the ACQUITY Column Manager method.
When a Waters 2777/Waters 2777C is used, users should use fill series to populate the vial reference. Using the "Add Samples" option beyond the maximum vial capacity could cause an application error in MassLynx.
Fill Series in the sample list does not work when using the Waters 2777/Waters 2777C with Alphanumeric Referencing.
Additional status can become blank after a power cycle of the Waters 25x5 pump. To recover, reinstall the ICS driver.
The first time an ACQUITY system is initialized, an error message about an ACQUITY server may appear. You may safely ignore this message.
When MassLynx and ICF drivers for GC 8890 and CTC PAL3 are installed on a fresh computer, the Inlet Editor status page 3777C/CTC PAL3 tab is blank. The workaround is to close the Inlet Editor and open it again.
If a method is created using PSI or Bar as the unit of pressure and later the unit is modified, the unit may not change on the Instrument Status page unless you close and then reopen the Inlet Editor.
In the GC Method Editor, when you click on the graphs in the "Instrument Method" tab, a crash dialog appears. Click **Continue** to work with the method. Click **OK** and then click **Save** on the Inlet Editor to save the method.

3777C/CTC PAL3
Do not add Priority samples when a job is present that uses Single Sample Overlap methods. If you want to add a priority sample, you must stop the currently running batch and add the priority sample.
Do not combine Single Sample Overlap and non-overlapping samples in a batch. CTC PAL3 enters an error state during a run if a batch is submitted with a mixture of "Single Sample Overlap" (Load Ahead) and "non-overlapping" inlet methods.
The instrument status page of Waters 3777C/CTC PAL3 may be blank after the initial MassLynx installation or after running the batch file to retrieve the CTC PAL3 Tool or Tray configuration. Close and then reopen the Inlets Method Editor.
If a run is aborted while the 3777C/CTC PAL3 is waiting for some condition to settle (for example, the Peltier stack to reach the desired temperature), the 3777C/CTC PAL3 will become unresponsive in the pre-inject state. Power cycle the 3777C/CTC PAL3 and re-establish communications.
You cannot prime the wash solvent using MassLynx. Use the handheld controller to prime the wash solvent.
The LC status OK indicator in the Inlet Editor does not correctly reflect the status of the system. When Reset communications is selected, the OK status indicator turns green before the 3777C/CTC PAL3 has completed its reset cycle. This can lead to a user starting a run before the 3777C/CTC PAL3 is ready, causing an error state. To solve this, reset communications again and wait approximately 40 seconds for the 3777C/CTC PAL3 to reset. Confirm 3777C/CTC PAL3 status in the "Waters 3777C" status tab before starting a run.
If you change the 3777C/CTC PAL3 configuration (for example changing plates or changing to headspace), to retrieve the new configuration from 3777C/CTC PAL3, close MassLynx. Run the ResetPAL3.bat batch file, which can be found on the Windows desktop, and then wait for about 40 seconds before reopening MassLynx.
In the **Autosampler** > **Instrument Configuration** > **Configure** window, the Retrieve Configuration and Tray Configuration buttons do not function. These functions are available via the PreConfigClient application.

Additional information

The following tables list additional information for SCN 1024.

Installation
When installing inlet drivers, it is recommended that you use the custom option to select and install only those components that you need.

Configuration

When a Waters 515 pump is used, you must ensure that the pump is connected and turned on before you turn on or reboot the Sample Fluidics Organizer (SFO)/ Pump Control Manager (PCM).

To control the eSAT/IN detector, you must install and use the Waters Pump Control driver.

On a 8890 GC, the headers shown on the Inlet Manager status tab (Column 1/Front inlets and Column 2/Rear/Back inlets) do not relate to the column numbers as set up on the Agilent GC.

On a 8890 GC, the readback values for column pressure and column flow for a column fitted to the rear inlet appear on the Inlet Manager status tab under the heading "Rear/Back inlets".

On a 8890 GC, the readback values for column pressure and column flow for a column fitted to the front inlet appear on the Inlet Manager status tab under the heading "Front inlets".

General

If you initiate a system startup to prime and equilibrate the BSM, and then stop the flow using any of the stop-flow icons, the prime function stops, but the equilibration function proceeds using the flow specified as the final condition.

When you perform a system startup using the ACQUITY console, the BSM seal wash does not automatically run. To run the BSM seal wash, select Control > Prime seal wash after the startup completes.

Extended wash is not supported for Waters 2695.

With a TUV or 2998 Detector, when a sample list acquisition is started, Chromatograms will show EI+ instead of the expected "Diode Array". However, this will be automatically corrected to "Diode Array" when the inlets start running.

On a 8890 GC, when you abort a sample list, the GC instrument continues to follow the oven program to ensure that no sample remains on the column. In this case, it is not possible to stop the GC using the software (for example, by using the Inlet Editor to reset communications or to load a new method). After aborting the sample list, tap the **Stop** button at the bottom-right of the GC instrument's touchscreen to stop the GC. To avoid possible data loss, allow the GC instrument to complete the current run before stopping it manually.

3777C/CTC PAL3

In the Autosampler window, the Pretreatment Method, Auxiliary Channels, and General tabs are not applicable to the 3777C/CTC PAL3.

After installing new firmware on the 3777C/CTC PAL3, create a new inlet method in order to ensure that the experimental record contains the latest firmware version number.

The Inject Cycle status indicator in the Inlet Editor does not correctly indicate the status of the inject cycle of the 3777C/CTC PAL3. With other systems on MassLynx, the Inject Cycle status indicator turns yellow during the injection cycle of the autosampler. The status never changes from gray when running a 3777C/CTC PAL3.

APPLICATIONS

Enhancements

The following table lists the software enhancements included in SCN 1024.

TargetLynx XS
You can now easily distinguish flagged samples using the new color-coding feature on the TargetLynx XS summary. A new column called "Summary Flag Reason" has also been added to the summary to detail the reason for highlighting.
It is now possible to flag samples that have high peak responses that fall above a quadratic calibration curve. The new flag field is called the OverCurve Flag. This flag enables a blank result caused by a very low response to be more easily differentiated from a blank result caused by a very high response – in both cases, the No Solution flag is triggered.
TargetLynx XS now applies the peak area or height threshold in proportion to the main peak. The expected ion ratio will be used to determine the threshold for a confirmatory ion peak.
You can now integrate chromatographic peaks using time increments of seconds rather than minutes. This new option in the TargetLynx XS Method Editor increases peak areas by a factor of 60.
You can now link a TargetLynx XS processing method with an acquisition method. Once linked, if functions in the acquisition method are added to or otherwise re-ordered, the function numbers in the processing method should be manually modified/adjusted to match the acquisition method.
TargetLynx XS now offers the ability to force a peak to be created with a fixed start and end retention time.
Mass columns are now available for use as additional concentration columns in the Method Editor. You can now set up to 50 independent concentrations.
The processing in TargetLynx XS in security mode is now significantly faster than before, especially when the raw data contains a large number of functions.
TargetLynx XS users can now add custom notes to results. Four plain text fields, four numeric fields, and four drop-down fields are available. Options in the drop-down fields are configurable. Custom notes are included in XML and TXT exports.
It is now possible to Print Preview results for a subset of samples, compounds, and groups.
Results for compounds reporting a blank concentration in TargetLynx XS can now be exported in the XML results file or uploaded using MassLynx LIMS Interface as either a blank or a zero. The default is a blank. To report a zero for all blank results, follow these steps: • In TargetLynx XS, open a .qld file and export the results to an XML file. This generates the registry key mentioned below.   • Open the registry editor (in the **Search** box, enter **regedit**, and then click on *regedit.exe*).

TargetLynx XS
• Go to *HKLM\Software\Wow6432Node\Micromass\TargetLynx*. • Locate the key "OutputBlanksConcAsZero". • Set the value to anything other than 0. • Restart TargetLynx XS.
The XML export time has been improved and the export will use less memory, allowing larger results files to be exported.
The exported XML results file is now displayed correctly in a text editor such as Notepad. Previously all the information would be on one line. The first row of the export now indicates encoding = "UTF-8".
The baseline end markers used to manually modify the peaks are now bigger.

Fault fixes

The following tables list the software problems fixed in SCN 1024.

General
If there were more than 29 channels in the MassLynx Chromatogram window, it was not possible to select all the channels and view them at once in the Chromatogram. This issue has been fixed.

IonLynx
When the IonLynx browser was opened to view results while a batch was processing, complete data for the last injection was not displayed or reported. This issue has been fixed.

Quanoptimize
In ESI mode, if you chose to optimize compounds in both Positive and Negative modes, the compounds were being optimized in a single injection, instead of data being acquired separately for each mode. This issue has been fixed.

TargetLynx XS
TargetLynx XS failed to process samples if the security UI was locked before the processing was completed. This issue has been fixed.
In MassLynx security, a mass Chromatogram could not be used to update the TargetLynx XS Method by clicking and dragging if the data file contained many functions. This problem has been fixed.

TargetLynx XS

When you opened the internal Method Editor from the TargetLynx XS browser and then exited the Editor after saving the changes, the focus did not return to the browser. This has been fixed.

In some scenarios, TargetLynx XS matched the confirmatory ion from an incorrect function. This has been resolved.

When the Method Editor was set up to update the Fourth Target Ion Parameters from the Chromatogram window, it updated the Third Target Ion Parameters instead. This has been fixed.

The "Don't Print Compounds Below Reporting Limit" option did not work for the Sample Template report. This has been fixed.

In MassLynx security, when switching between the compounds in the TargetLynx XS Method Editor, sometimes the wrong compound was highlighted. This issue has been fixed.

The Blank subtract concentration was incorrect if a solvent was present between blanks. This issue has been fixed.

In the TargetLynx XS browser, when displaying the chromatogram with confirmatory ions, sometimes the wrong ion trace was displayed. This issue has been resolved.

In the TargetLynx XS method, under **Integration parameters** > **Apex Track**, you could set the Baseline Start or End threshold (%), click **Save**, and then print the method. But if you reopened the method, you sometimes found that the set values were rounded. This fault has been fixed.

The LOD was not being exported in the XML results file for samples with no concentration calculated. This issue has been fixed.

The peak areas and heights were not exported to XML for deleted peaks. This has been fixed.

When you placed text in the SPARE_1 to SPARE_5 columns, processed the samples in TargetLynx XS, saved the dataset, and exported the results to the LIMS txt file, the information was correctly exported in the Header for each sample in the txt file. However, if you closed and reopened the dataset and then exported the results to a LIMS text file, the Spare 1-5 fields were empty. This has been fixed.

For results that would have triggered the no solution flag, the flag is no longer set when the peak is deleted or when no peak is found.

The Front Width, Tail Width, and Peak Asymmetry values rounded incorrectly when saved. This has been fixed.

Sometimes, not all compounds were transferred to TargetLynx XS by POSIT+VE. This problem has been fixed.

The ability to modify a TargetLynx XS method file and click **Save** required the Windows delete permission for the desktop user. This has been fixed. The required Windows permissions are now Read, Write, and Execute.

The Job information from the raw data file was not displayed in the header of either the sample summary report or the samples report. This has been fixed.

In the Print dialog, the maximum number of characters that could be entered into the Samples, Compounds, and Groups fields was limited to the visible length of the field. This has been fixed.

TargetLynx XS

Occasionally, a TargetLynx XS QLD file could become read-only when you tried to save it to a shared network folder. This issue has been corrected.

Quan Ions were not extracted during TargetLynx XS processing of isobaric MRMs if the masses in the experimental method had four decimal places. This fault has been fixed.

TargetLynx XS results were sometimes flagged in red in the Overview table for no apparent reason. This was due to the flagging of peak asymmetry where the Quan ion passes but a confirmatory ion fails. This issue has been fixed.

OpenLynx

An issue with OAToolkit not copying lists of OpenLynx methods between OALogin instances is now fixed.

An issue with user information not correctly transferring between OALogin and OAToolkit is now fixed.

The information such as File Name, Sample Description, and so on were not being transferred to failed sample OLB file produced by OpenLynx. This issue has been fixed.

TrendPlot

TrendPlot now displays the mean as a number as well as a line.

TrendPlot did not distinguish between different compounds if the first parts of the compound names were similar. This problem has been fixed.

MassLynx Security

MassLynx now records an audit event on deleting a raw data file via the Chromatogram browser.

The MassLynx Security Manager prompted for save even though no changes were made. This has been fixed.

LogLynx failed while scrolling through events if a single event was greater than 128 kB in size. This issue has been fixed.

In MassLynx Security, users in the Maintenance Group were unable to import files. This has been fixed.

In MassLynx Security, when multifunction data were displayed in the MassLynx Chromatogram window, some chromatogram traces did not appear. This issue has been fixed.

Quanpedia

Quanpedia can now create secure method files when full security is installed.

Concessions

The following tables list the known software issues for SCN 1024.

TargetLynx XS
Do not rely on the units in the concentration column header in report tables that show results from multiple compounds.

Quanpedia
When a Quanpedia database is opened on a computer from a shared location and the same database is opened from another computer, no error is displayed informing the users that the database is already open.

QuanOptimize
TargetLynx XS processing can fail due to a mismatch in the function numbering of data obtained via a specific QuanOptimize setup. When the lowest mass compound optimizes in negative mode, it is placed in function 2 of the MS Method but assigned Function 1 in the TargetLynx XS method. Positive compounds are acquired in function 1 but assigned function 2 in the TargetLynx XS method. This causes a failure in the AutoQuantify option and in all subsequent TargetLynx XS processing. To avoid this issue, do not use the AutoQuantify option. Manually correct the functions in the TargetLynx XS Method.
When performing a QuanOptimize Analysis, MassLynx describes the PreOptimize and PreAnalysis stages as Running Loop Switching Method and Running Column Switching Method, respectively.

IonLynx
The highlighted combined area in the graphical display in the IonLynx results browser window sometimes does not display correctly. This is an intermittent issue that does not persist when scrolling back and forth through the sample sequence. The processed data are unaffected regardless of the graphical display. Scroll to the next or previous sample then back to the sample in question, or re-size any of the browser panes within IonLynx.

Additional information

The following table lists additional information on concessions for SCN 1024.

TargetLynx XS
If you delete a function in a linked MS Method and don't update the TargetLynx XS method, you will see a blank results page for that compound. To resolve this issue, remove the corresponding function from the TargetLynx XS method manually and process the data.

TargetLynx XS
You can configure the custom selection fields with options of up to 119 characters. However, lengthy text may not be completely displayed when you are annotating a result. If this is the case, use the column editor to reduce the length of the text for any options that appear ambiguous.

Supported hotfixes and antivirus software

The following updates on Windows 10 Enterprise LTSB 1607 are supported with MassLynx version 4.2 SCN 1024:

Description	Hotfix ID
Update	KB4589210
Update	KB4033393
Update	KB4049411
Update	KB4033631
Update	KB4132216
Security Update	KB5005043
Security Update	KB4535680
Security Update	KB5001402

Note: Windows updates will sometimes re-enable the PC firewall. After every Windows update, inspect the firewall to verify that it remains disabled.

Antivirus

SCN 1024 was tested with Cortex XDR version 7.1.0.45682. Search support.waters.com for advice on configuring other AV software for use with MassLynx.