MassLynx™ 4.2
SCN 977
Release Notes

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MassLynx Software Change Note #977

Introduction:

MassLynx Software Change Note #977 provides support for the Waters Xevo TQ-S micro Detector and it supersedes SCN 945 and SCN 960. This software change note includes new enhancements, fault fixes and concessions (including all the concessions from superseded SCN 945 and SCN 960) as described in the Enhancement, Fault Fixes and Concessions sections of this document. MassLynx 4.2 SCN 977 introduces support for Windows 10 Enterprise LTSB.

Included Drivers:

The MassLynx 4.2 SCN 977 installation includes the following drivers:

MS	SCN Version
Xevo TQ-S micro	SCN 977

LC / Inlets	ICS Version
Waters Driver Pack 2017 Release 1	Waters Driver Pack 2017 Release 1
GC - Agilent 7890	2.02

Supported Components:

The MassLynx 4.2 SCN 977 installation supports the following drivers. For configuration recommendations, please contact your local Waters specialist.

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 Convergence Manager
ACQUITY UPC^2 BSM
ACQUITY Auxiliary Solvent Manager
ACQUITY µBinary Solvent Manager
ACQUITY µBinary Sample Manager-FL
ACQUITY Sample Organizer
ACQUITY Trap Valve Manager
ACQUITY HDX Manager
Waters Pump Control
Waters 2996 PDA
Waters 2695 (controlled via GPIB)
eAlliance - controlled via GPIB
Acquity Online SPE Manager
Agilent 7890

Operating Systems:

MassLynx 4.2 SCN 977 is supported on English version of Microsoft® Windows® 7 Professional 64-bit, Service Pack 1 on a Waters-supplied acquisition workstation.

MassLynx 4.2 SCN 977 is also supported on English version of Microsoft® Windows® 10 Enterprise LTSB 1607 on a Waters supplied Lenovo P520 only.

Security:

Basic and Full MassLynx security configurations are supported.

SCN 977 Installation Procedure:

MassLynx 4.2 SCN 977 is a complete installation of MassLynx 4.2. If any other MassLynx SCNs are already installed they must be uninstalled, by using the Windows 'Programs and Features' facility in the Windows Control Panel, before installation of MassLynx 4.2 SCN 977.

1. Close MassLynx and any other software applications.
2. If any instrument drivers - such as ACQUITY drivers, Waters 2777 / CTC drivers - have been installed they must be removed, by using the Windows 'Programs and Features' facility in the Windows Control Panel, before installing SCN 977.
3. Waters Pump Control should be removed via the deployment manger prior to MassLynx installation.
4. If MassLynx is installed, it should be removed, by using the Windows 'Programs and Features' facility in the Windows Control Panel, and the PC should be rebooted after the removal is complete.
5. Manually delete the "C:\Program Files (x86)\Micromass Utilities\ICOP" folder prior to installation of SCN 977.

Install MassLynx V4.2 SCN 977 following the installation instructions.

1. Select Start–>Run from the windows start menu and type:
   - <DVD–Drive>:\setup <return>
   - Where, <DVD–DRIVE> is the drive letter of the DVDROM.
2. Follow the instructions within the installation wizard.
3. Click Finish to complete installation of the SCN files.
4. Reboot the PC and log back into Windows.
5. Reboot the instrument embedded PC if MassLynx was installed with Xevo TQ-S micro option selected during installation.

If an inlet system is being used:

1. Launch MassLynx and open the Inlet Editor. Select "Instrument Configuration…" from the Tools menu
2. Install any required Waters instrument drivers (ICS) using the Deployment Manager by clicking "Setup Instruments". If any drivers are installed it is recommended that the PC is rebooted afterwards before continuing the inlet system configuration.
3. Click "Configure" to launch the Inlet Configuration Dialog to complete the configuration of the inlet system

Note: **Modifying or repairing an installation is not supported**.

Note: OpenLynx is included on all installations of SCN 977.

Note: Instructions for installing the ACQUITY Components can be found in the 'Installing ACQUITY Driver Components' section, this will include configuration of the Isocratic Solvent Manager.

The ICS for M-Class support are not provided on the SCN 977 DVD. The requisite ICS needs to be installed from the respective disk provided with the ACQUITY ionKey instrumentation

Installation of Stand–Alone Applications

This instruction is for installation of OALogin, OAToolkit, OpenLynx Browser and TargetLynx Browser.

If any of these applications are already installed they must be removed, by using the Windows 'Programs and Features' facility in the Windows Control Panel, before installing the SCN 977 version.

1. Close any open software applications.
2. Insert the MassLynx SCN 977 DVD into the DVD–ROM drive.
3. Navigate to the Applications folder on the DVD 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 installation of the SCN 977 files.

Installation of Quanpedia databases

Example databases are available on a separate CD. These example databases should be copied onto the PC and can then be opened in Quanpedia by selecting Options | Database | Open.

Files copied from a CD may have the read-only flag set and this will need to be removed.

To manually remove the read-only attribute from a file:

1. In Windows Explorer, right-click the file that you want to change, and then click Properties.
2. On the General tab, click to clear the Read Only check box.

Click OK.

Adobe Print Driver Setup

"Print to PDF" options in MS Console and MS Method Editor require the Adobe PDF print driver to be installed. This driver is part of Adobe Acrobat Distiller, which is included in Adobe Acrobat Professional. The recommended and validated version of Acrobat Professional to work alongside MassLynx is Adobe Acrobat Professional 9.0. Please install this version of Acrobat Professional before attempting to use MassLynx "Print to PDF" options.

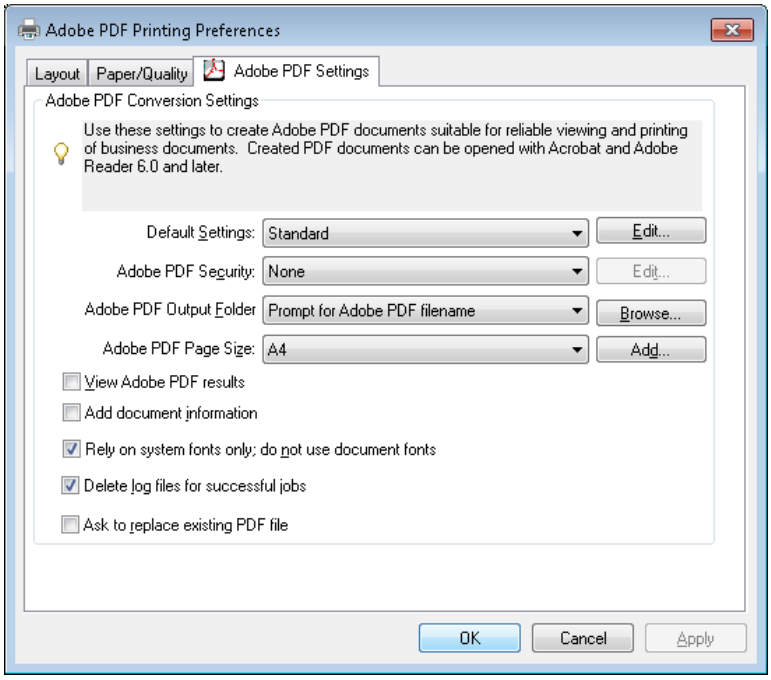
Software setup:

- Log in as an administrator and install 'Adobe Acrobat 9' using the default setup options. A restart may be required.
- Once installation is complete, double click the 'Adobe Acrobat 9 Standard' link on your desktop.
- Read and accept the license agreement, then close the 'Adobe Acrobat' window.

The following steps apply to each user account on the host PC:

- View installed printers from the Windows Control Panel.
- Ensure 'Adobe PDF' is listed - do not alter its name.
- It is recommended that 'Adobe PDF' is not selected as the default printing device.
- Right click on 'Adobe PDF' and select 'Printing Preferences'.
- On the 'Adobe PDF Settings' tab, ensure the following options are selected:
    - Default Settings: Standard
    - Adobe PDF Security: as appropriate
    - Adobe PDF Output Folder: Prompt for PDF filename
    - Adobe PDF Page Size: as appropriate

- Ensure only the following boxes are checked:
    - Rely on system fonts only; do not use document fonts
    - Delete log files for successful jobs



- Press Apply and OK

Note: To configure PDF printing for OALogin, the 'Adobe PDF Output Folder' must be set to the OALogin ReportDB directory (normally C:\MassLynx\OALogin\ReportDB).

Un-installation:

MassLynx can be removed by using the Windows ‘Programs and Features’ facility in the Windows Control Panel.

MS

General Note(s): SCN 977 is for the Xevo TQ-S micro detector. It supersedes SCN 945 and SCN 960.

Enhancements:

The following table contains a list of software features included in SCN 977

Support for UniSpray source.

Fault Fixes:

The following table contains a list of software problems fixed in SCN 977

With an IonKey source, it was not possible to use Intellistart routines. This issue has been corrected.
Tune page is locked down when a Sample list acquisition is in progress. This prevents users from modifying the settings when running an acquisition.
An issue with function ordering has been corrected in Method Editor. The functions are now correctly ordered.
An issue with Interscan delay has been fixed when multiple MS2 scan functions were in a method.

Concessions:

The following table contains a list of known software issues and workarounds for SCN 977

General
The license revision displayed during SCN Installation wizard is incorrect. The correct license revision can be found in the customer hard copy.
If utilizing a TargetLynx Processing method, after modifying and saving acquisition methods in an associated MS Method, please ensure that the ordering of the functions in MS Method Editor matches with the ordering of functions in TargetLynx Processing method file
MassLynx will hang if user selects “Network” from the “Print Setup” dialog box. Printers must be configured in the operating system first, as they will then be available in MassLynx “Print Setup” without needing to click “Network”.
By design a non-admin user cannot adjust date and time settings.
By design, MassLynx does not support “User switching” option of Windows. When switching between users, User should logoff and then log back in as other user.
Non OS Admin users cannot run ACQUITY Plot Viewer from C:\Program Files (x86)\Waters Instruments\Bin folder.
To install ICS instruments older than 1.4 the ICSCompanionSetup.exe should be run manually.
It is recommended that if removing some ICS instruments and not replacing with others, then the ICS should not be removed, the instruments should only be de-configured from MassLynx and the console.
Careful consideration should be given when setting up shut down 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.
On rare occasions during the install, an error message is displayed stating that the DHCP Server failed to register. If this message is seen, the installation should be cancelled and then started again.
On rare occasions during an uninstall of MassLynx, an error message is displayed stating “Waters DHCP error - 'Could not delete service"'. If this message is seen it should be acknowledged and after the process has completed the PC should be rebooted before attempting a further install.
A sample list batch cannot be modified once it has been submitted.
Desktop only install – an incorrect error message stating "Failed to create new project" will be displayed when creating a new project, it can be ignored as the project will be created as required.
When switching MassLynx projects the sample list browser may occasionally open in the incorrect project, users

should browse to the required project if this occurs.
All ESCi experiments should be run in the ESCi ion mode, not the ESI Ion mode.
Shutdown tasks “Source Gas On” and “Source Gas Off” options are only present after starting an acquisition with IntelliStart.
In dual polarity experiments, the experiment report will show all ‘actual’ readbacks in the polarity of the last active function.
When running with a security enabled system you may be required to reboot the instrument PC prior to opening MassLynx Security Manager. Upon opening MassLynx Security Manager you may be warned that MassLynx applications are currently running. Reboot the windows PC to enable access.
When first connecting the NanoFlow source USB camera a dialog will appear to request the location of the camera driver. The camera driver is located in the c:\Masslynx\USBCameraDriverForWindows7.
When first utilising the ionKey USB camera, the camera configuration window will be displayed. Selecting the ‘USB’ option with defaults will no longer display an image. The following settings are required to give an image; Video Norm: Pal_B Video Format: Y800 (768x576) Frame Rate: 25. Imput Channel: 00 Video:Composite
Initial Conditions Method Events Reservoir Selection does not switch Reservoirs correctly, instead a timed method event should be utilised.

Tune Page
Sporadically, when changing ion mode, the instrument may not switch to the correct polarity. Reinitialising the instrument will correct this issue.
After linking a calibration to a tune file within the tune page the tune file must be saved before the link is permanently stored.
When altering the Smooth Window parameter in the Instrument Threshold menu ensure the dialog is closed before closing MassLynx for the value to be retained.
If the instrument is switched to Standby during the running of the Detector Gain Wizard, the wizard should be stopped and restarted once back in Operate.
When utilising an ESCi source, to view accurate tunepage readbacks all functions should utilise the same mode in the tune page display.
When utilising an ionKey source, to utilise a TriZaic tile the user should still select the ionKey source tab and alter the defaults as required for the TriZaic tile.
After switching ion mode the toolbar can occasionally appear to be disabled (greyed out), highlighting the toolbar options or navigating away from the tune page will correct this occurrence.
If changing the source whilst in operate it is recommended that the instrument is switched into standby and back to operate once the new source is fitted to ensure the source ID updates.
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.

Console / IntelliStart
The console needs to finish loading before any options are selected. Closing the console before this point can cause it to enter into an error state.
Occasionally when opening the console for the first time, the console plots will not display. Closing and reopening the console will display the plots as expected.
The console plots can occasionally fail to update, the instrument data collection is not affected and the plots will resume as normal after a short period.
Clicking between the ACQUITY log entries can cause an error in the Console.
Cancelling a print of the ACQUITY logs can cause an error in the Console.
Printing from the ACQUITY logs will print all entries, to print a single log, it should first be printed to PDF and then the relevant log selected.
When utilising an ionKey source all IntelliStart functionality is only supported for the positive ion mode.
The Rear Panel pages inject start indicator will not update on contact closure, Event In 1 will be indicated via the

Event In display, Event In 2 is not shown.
The automatic filename qualification in Sample Tune Develop Method can occasionally not populate the file path correctly when opening a tune page IPR file from a different project.
When running IntelliStart in a secure MassLynx system, the project folder utilised should have full deletion rights. It is recommended that the, user defined, generated ipr, experiment and report files are stored in a separate results project.
Before importing existing projects into a secure install of MassLynx, the raw data files should be removed from the project.
In a secure MassLynx system, an IntelliStart sequence will not generate any reports if the security timeout locks the system.
In a secure MassLynx system, creating a new Sample Tune file via IntelliStart without the permission 'Tune Page – Alter Tune File' will enact an incorrect error dialog regarding permissions. Clicking OK on this message will allow the IntelliStart sequence to continue.
When utilising IntelliStart, deleting the currently selected analysis from outside of the console will cause the console to error.
In IntelliStart, the advanced setup resolution and calibration Mass Range selected must encompass at least four masses present in the selected reference file.
Factory default resolution parameters will be loaded and checked during a resolution sequence which has a target resolution of less than 0.75 Da, unless specifically overridden for each run through the advanced options.
If utilising IntelliStart with a NanoFlow source, the user must ensure that a stable beam is present before starting the IntelliStart sequence.
Prior to running IntelliStart calibration pre-check, it is advisable that the user check the signal intensity of their masses of interest prior to running the check, ensuring that the correct cone voltage is selected for the calibration compound in use.
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\
It is advisable that the users check their mass of interest with the calibration check previously performed to ensure that the peak is not too close to the acceptance window. Also users should check that the cone voltage has been applied correctly if the beam check failed.
IntelliStart Calibration will always calibrate in the following order: static, dynamic, fast scanning. This is also the order in which the report 'save as' dialog boxes will be presented during the calibration.
Do not schedule an LCMS system check to run when another LCMS system check is going to still be active.
If running a LC/MS System Check, this will need to be performed after any previous submitted batch has completed.
Manually changing the calibration file linked to a resolution file created via an IntelliStart analysis will not be recognised by the IntelliStart system. Upon reselecting the analysis type via the console, IntelliStart will continue to utilise the original linked calibration file.
Closing and reopening the console during an IntelliStart sequence will result in IntelliStart not recognising the sequence or its results once it completes.
OpenLynx must be installed for the IntelliStart LCMS System Check feature to function.
When using an LC system with IntelliStart, it is essential that the system is configured within the Inlet Editor prior to the IntelliStart run. The IntelliStart system will fail to adjust the desolvation temperature and gas flow if the LC system is not configured.
For IntelliStart LC/MS System Check to be completed for both positive and negative ionisation modes the individual analysis needs to be executed separately.
Prior to running a LC/MS System Check, ensure the vial inputs are correctly assigned.
When MassLynx is closed and re-opened, IntelliStart will revert to saving files and methods in the 'default.pro' Project directory. The required project needs to be re-opened in MassLynx for IntelliStart to save to the correct location.
The save option associated with a report produced by QC check does not work. As such, it is not possible to rename the file and save elsewhere. Users need to record the file name and generation time in order to return to it at a later date. Alternatively it can be printed upon generation.
The two ISD checks "LC/MS System Check Has Not Been Performed" and "LCMS System Check Failure" have a higher priority than many of the other IntelliStart checks. In order to see these other IntelliStart checks, the two higher priority checks can be disabled by de-selecting the relevant option via the Configure > IntelliStart Configuration menu.
When setting up a LC/MS system check to check the retention time window, 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 upon the largest peak in the chromatogram.
To stop LC/MS system check once started, go to the MassLynx sample list and press stop then go to the inlet page and press the stop hand.
If you are running a LC/MS system check in an opposite polarity to the tune page the experiment utilised should contain at least one function in the polarity of the tune page.
The experiment utilised to conduct LC/MS system check should not contain both scanning and static functions, i.e. only SIR/MRM or scanning, not mixed mode.
If a LC is not present in the system, the ISD checks relating to LC/MS, LC/MS System Check Has Not Been Performed" and "LC/MS System Check Failure", should be removed from the system.
Smoothing is disabled by default in System QC OLP files.
Entering the characters * / \ ? as part of names or filenames in IntelliStart will cause an error. If the error is triggered click continue and rename the file using valid characters.
If the lamp parameter has been set to 'off' as a task during IntelliStart System Startup, the instrument will also go out of operate when the lamp turns off.
When using the multiply charged function, within 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 product ion 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 2048m/z).
When running a multiple compound Sample Tune Develop Method, if any of the transitions are not found the report generation can occasionally fail which will display an ‘Internal Error’ message in the console. Restarting the console will remove the error message and it is recommended in these instances to utilise single compounds to achieve the desired results.
When running a multiple polarity Sample Tune Develop Method, if the most intense optimised transitions all reside in a single polarity, then only this polarity will be utilised to generate methods. Running single polarity Sample Tune Develop Methods will avoid this issue.
When running a multiple polarity Sample Tune Develop Method, the overall process will return as passed if one of the polarities successfully completes. In this scenario a health check will activate to indicate which polarity didn’t complete as expected.
IntelliStart Sample Tune Method Develop filenames should be restricted to a maximum of 210 characters to allow future editing via the Method Editor.
When utilising an ESCi source to perform ES only Sample Tune Method Develop ensure that the APCi probe temperature matches the Desolvation temperature required. The APCi Probe temperature can be set via the APCi Tune Page.
The Intellistart Sample Tune Method Develop Combined infusion syringe flow rate is not automatically set dependant on the Acquity flow rate, it is defaulted to a value of 10ul/min. This default may not produce a stable beam at high LC carrier flow rates.
If a sample tune file that has been generated by IntelliStart is overwritten at any point then the error message "sample tune is invalid" will occur.
The IntelliStart Sample Tune sequence must be utilised to obtain a parameter file that contains the resultant optimised instrument parameter settings and linked calibration parameters produced by the IntelliStart Resolution and Calibration sequences.
To avoid the calibration screen continually prompting for user input when printing to file it is recommended that Adobe Professional is utilised and the option 'Print to PDF' be utilised instead of 'Print' - this will automatically produce PDFs in the IntelliStart.PRO folder and does not require user input.
In order to use the Waters 2777 Autosampler with the IntelliStart LCMS System Check in regulated Full Security mode, the following steps need to be carried out: 1. Copy all files from <MassLynx>\Default.PRO\ACQUDB\ to <MassLynx>\SystemQC.PRO\ACQUDB\ ensuring existing files in the destination directory are not overwritten. 2. In MassLynx, log in as a regulated user, select to ‘Import Project’ and choose the SystemQC.PRO folder – this will generate checksums for the copied files. 3. LCMS System Check will now work as expected
Manual Optimisation should only be utilised after a successful Sample Tune Method Develop.
To be able to run IntelliStart setup in Basic Security, users must have the ‘overwrite RAW data’ permission enabled.
In Full Security regulated mode, HTML reports are now deleted following the completion of a resolution setup and a

sample tune develop method. In unregulated mode, the software includes an option to retain the HTML reports.

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

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

Key ● 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
When running with a security enabled system it is recommended to limit experiments to a maximum of 250 MRM functions with 32 channels or 50 SIR with 32 channels. Execution of experimental methods with more than 32 functions with security will result in a drop in system performance.
Method Event initial settings should be used for events which are to occur at a time 0.0, if the required event is not available in the initial settings it should be set to a time of 0.01.
Enabling and disabling the MRM/SIR V-Sort algorithm can take up to 3 minutes if the experiment contains a large number of functions.
When using MassLynx to record PDA or TUV channel data, a maximum of 1023 functions should be utilised in the Method Editor.
If an MS Method was created on a previous version of MassLynx, the user should open the file in Method Editor and re-save the file before running on the instrument. This will ensure the experiment's functions will be run in the order shown in Method Editor.
When using the Phosphopeptide method, it is recommended that a calibration is performed over the full mass range (2-2048Da).
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."
Precursor Ion mass is set at zero in a phosphopeptide analysis experiment when viewed from the Chromatogram. The Precursor Ion Mass can be found manually in the _PPPT.txt report.
When setting up timed events involving fluidics care should be taken to ensure scheduled events are giving enough time for each operation to complete. Attempting a fluidics timed event while a previous fluidics timed event is still

in operation may result in non execution of the later event.
When creating methods the following error message may be seen "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?" Not selecting automatic update of dwell times may result in a reduction of instrument lifetime.
When creating method events, there should not be any events in between the solvent delay start event and the solvent delay end event.
When creating a SIR function, the Undo, Redo and Clear all buttons do not have an effect on the Auto Dwell entries.
When changing the default PIC parameters via the drop down menu, all MRM functions which contain PICs should be opened and saved to ensure the parameters have been applied correctly.
We recommend the use of short scan times for both the 'Switch From' and 'Switch To' functions when running Survey Functions. Use of long scan times reduces performance when switching between functions.

INLETS

Concessions:

The following table contains a list of known software issues and workarounds for SCN 977.

General
If utilizing a TargetLynx Processing method, after modifying and saving acquisition methods in an associated MS Method, please ensure that the ordering of the functions in MS Method Editor matches with the ordering of functions in TargetLynx Processing method file.
When installing Inlet drivers it is recommended that users utilise the custom option to allow them to deselect the ACQUITY components which are not supported by this instrument (see Supported Products/Configurations & Installing ACQUITY Driver Components sections), rather than utilising the default option which is to install all drivers.
During inlet configuration, Waters deployment manager does not automatically launch when required. Each ACQUITY component should be setup manually before configuring them in the inlet editor using the "Setup Instrument" button in the inlet configuration window.
When installing components via the Inlet Editor, the ACQUITY Console should not have previously been opened since the PC was restarted. Users should restart the PC and then install new components without opening the Console before installation.
It is recommended that users do not use a higher scan rate than 1 scan per sec with the Waters 2996 detector.
When running ACQUTY Open Architecture System, the column temperature data channel should be enabled in the ACQUITY Column Manager method.
'Fill Series in the sample list does not work when using the Waters 2777 with Alphanumeric Referencing'.
The first time an ACQUITY system is initialized an error message about an ACQUITY server may pop up. This can be safely ignored.
Waters Pump Control should be removed via the deployment manger prior to the removal of MassLynx.
When a Waters 515 is used, users must make sure that 515 pump is connected and turned on before the SFO/PCM is turned on or rebooted.
Extended wash for Waters 2695 and 2795 is not supported.
eSatin detector will need to be installed with Waters Pump Control ICS driver.
eSatin channel description is only saved when selecting the "x" to close the method editor.
If there is not a Default.esat method in the project Acqudb folder, new eSAT/in methods cannot be created. A Default.esat method is provided in the Default project when MassLynx is installed. It can be copied to any new project that does not have this file.
Waters 2545 pump is shown as Waters 2535 in the experimental record.
When a Waters 2777 is used, users should use fill series to populate the vial reference. Using "Add" sample beyond the maximum vial capacity could cause application error in MassLynx.
Additional status can become blank after a power reboot of the Waters 25x5 pump. Re-installing the ICS driver is advisable in order to recover.
With a TUV or 2998 Detector, when a Sample list acquisition is started, Chromatograms will show EI+ instead of expected "Diode Array". However, this will be automatically corrected to "Diode Array" once the inlets starts running.

APPLICATIONS

Enhancements:

The following table contains a list of features added in SCN 977.

TargetLynx
TargetLynx XS now offers the ability to keep manual peak modifications over consecutive reintegrations, providing there are no modifications to the TargetLynx XS Method for settings affecting integration and extractions. This also includes the number of compounds and names in the method.
TargetLynx XS now offers the ability to set retention time tolerance in the TargetLynx XS method as absolute values, rather than just percentage.
TargetLynx XS now offers the ability to report samples below a concentration threshold by setting a minimum standard addition concentration value in the concentration flagging section of the TargetLynx XS Method Editor.
Quanpedia now allows users to update compound retention times within an analysis using QLD files generated by TargetLynx XS.

Fault Fixes:

The following table contains a list of software problems fixed in SCN 977.

TargetLynx
TargetLynx XS now displays flag tips after saving and reopening QLD files.
TargetLynx XS reports no longer display MassLynx twice in report titles.
TargetLynx XS now raises the Ion Ratio flag in the even the target ion is missing.
TargetLynx XS now allows the users to open QLD files from network locations.

ChromaLynx
An issue with reading data where the mass are intensities greater than ~1xE9 has been corrected.

Concessions:

The following table contains a list of known software issues and workarounds for SCN 977.

TargetLynx
A TargetLynx .QLD file will become locked when saved to a folder for which the Windows user does not have the Windows Modify permission
A modified calculated concentration column header will not be reflected in the samples report, it will remain with its default heading.
The following values will be blank when the indeterminate flag is set:- Calculated Concentration % deviation % Recovery LOD Flag LOD LOQ Flag LOQ

Processing 2048 functions data (1024 MRMs and 1024 PICs) can take upto 10 minutes to complete.
An issue was identified with the “Keep Peak Modifications” feature in TargetLynx XS. Manual peak modifications aren’t cleared if the user only enables / disables the “Apex Track Enabled?” option in the Integration section.
As with previous releases of TargetLynx (XS), in the event a peak is thresholded out during integration / quantitation, the No Solution flag may still be triggered for a sample.
In the event the Calculated Concentration field is blank within the TargetLynx XS browser summary pane and/or chromatogram window, the “analconc” field is now exported in either XML / TXT files or MassLynx LIMS Interface v3.0 as a blank. Please review the data for any blank concentrations in the Calculated Concentration field

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
Pressing F1 to access help is not implemented for the following QuanOptimize applications (it can still be accessed by the main menu): Edit Method Run QuanOptimize View Results
It is recommended that QuanOptimise is only utilised for a single polarity per analysis.
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 all subsequent TargetLynx XS processing. To correct this issue, the AutoQuantify option should not be utilised and the functions must be manually corrected in the TargetLynx XS Method.
When performing a QuanOptimize Analysis, MassLynx describes the ‘PreOptimise’ and ‘PreAnalysis’ stages as ‘Running Loop Switching Method’ and ‘Running Column Switching Method’ respectively.

Supported Hotfixes and Anti-Virus software:

The following Windows Updates are supported with MassLynx v4.2 SCN 977:

Windows 7.0 64 Bit Professional SP1

Description	HotFix ID	Description	HotFix ID	Description	HotFix ID
Update	KB2849697	Update	KB2563227	Security Update	KB2698365
Update	KB2849696	Security Update	KB2563894	Update	KB2699779
Update	KB2841134	Security Update	KB2564958	Security Update	KB2705219
Update	KB2670838	Security Update	KB2567680	Security Update	KB2706045
Update	KB2830477	Update	KB2570791	Update	KB2709630
Update	KB2592687	Security Update	KB2570947	Update	KB2709981
Update	KB971033	Update	KB2574819	Security Update	KB2712808
Security Update	KB2393802	Security Update	KB2579686	Security Update	KB2716513
Security Update	KB2425227	Security Update	KB2584146	Update	KB2718704
Security Update	KB2476490	Security Update	KB2585542	Security Update	KB2719033
Security Update	KB2479943	Update	KB2603229	Update	KB2719857
Update	KB2484033	Security Update	KB2604115	Security Update	KB2719985
Update	KB2488113	Update	KB2616676	Security Update	KB2724197
Security Update	KB2491683	Security Update	KB2618451	Update	KB2726535
Update	KB2492386	Security Update	KB2619339	Security Update	KB2727528
Hotfix	KB2496898	Hotfix	KB2619497	Update	KB2729094
Security Update	KB2503665	Security Update	KB2620704	Security Update	KB2729452
Update	KB2505438	Security Update	KB2620712	Update	KB2731771
Update	KB2506014	Security Update	KB2621440	Security Update	KB2731847
Security Update	KB2506212	Security Update	KB2631813	Update	KB2732059
Update	KB2506928	Update	KB2640148	Update	KB2732487
Security Update	KB2507618	Security Update	KB2644615	Update	KB2732500
Security Update	KB2509553	Security Update	KB2645640	Update	KB2735855
Update	KB2511250	Security Update	KB2647518	Update	KB2736233
Security Update	KB2511455	Update	KB2647753	Security Update	KB2736422
Update	KB2515325	Security Update	KB2653956	Update	KB2739159
Update	KB2522422	Security Update	KB2654428	Update	KB2741355
Update	KB2529073	Security Update	KB2655992	Security Update	KB2742599
Security Update	KB2532531	Security Update	KB2656356	Security Update	KB2743555
Update	KB2533552	Security Update	KB2656411	Update	KB2749655
Update	KB2534366	Security Update	KB2658846	Update	KB2750841

Security Update	KB2536275	Security Update	KB2659262	Security Update	KB2753842
Security Update	KB2536276	Update	KB2660075	Update	KB2756822
Update	KB2541014	Security Update	KB2660649	Security Update	KB2756921
Security Update	KB2544893	Update	KB2661254	Security Update	KB2757638
Update	KB2545698	Security Update	KB2667402	Security Update	KB2758857
Update	KB2547666	Security Update	KB2676562	Update	KB2761217
Hotfix	KB2550648	Update	KB2677070	Update	KB2762895
Update	KB2552343	Update	KB2685811	Update	KB2763523
Security Update	KB2555917	Update	KB2685813	Security Update	KB2769369
Security Update	KB2556532	Security Update	KB2685939	Security Update	KB2770660
Security Update	KB2559049	Security Update	KB2688338	Update	KB2773072
Security Update	KB2560656	Security Update	KB2690533	Security Update	KB2778930
Security Update	KB2562937	Security Update	KB2691442	Update	KB2779562
Security Update	KB2785220	Security Update	KB2861698	Update	KB2923545
Update	KB2786081	Security Update	KB2861855	Update	KB2928562
Update	KB2786400	Security Update	KB2862152	Update	KB2929733
Security Update	KB2789645	Security Update	KB2862330	Security Update	KB2931356
Security Update	KB2790113	Security Update	KB2862335	Security Update	KB2937610
Update	KB2791765	Security Update	KB2862966	Security Update	KB2939576
Update	KB2798162	Security Update	KB2862973	Security Update	KB2943357
Update	KB2799926	Update	KB2863058	Update	KB2952664
Update	KB2800095	Security Update	KB2863240	Security Update	KB2957189
Security Update	KB2803821	Security Update	KB2864058	Security Update	KB2957509
Security Update	KB2804579	Security Update	KB2864202	Security Update	KB2961072
Security Update	KB2807986	Security Update	KB2868038	Security Update	KB2965788
Update	KB2808679	Update	KB2868116	Update	KB2966583
Security Update	KB2813170	Security Update	KB2868623	Security Update	KB2968294
Security Update	KB2813347	Security Update	KB2868626	Update	KB2970228
Security Update	KB2813430	Security Update	KB2868725	Security Update	KB2972100
Update	KB2813956	Security Update	KB2871997	Security Update	KB2972211
Security Update	KB2820197	Security Update	KB2872339	Security Update	KB2972280
Update	KB2820331	Security Update	KB2875783	Security Update	KB2973112
Security Update	KB2830290	Security Update	KB2876284	Security Update	KB2973201
Security Update	KB2832414	Security Update	KB2876315	Security Update	KB2973351
Security Update	KB2833946	Security Update	KB2876331	Security Update	KB2977897
Update	KB2834140	Update	KB2882822	Security Update	KB2977292
Security Update	KB2834886	Security Update	KB2883150	Security Update	KB2978120

Security Update	KB2835361	Security Update	KB2884256	Security Update	KB2979570
Security Update	KB2835364	Security Update	KB2887069	Security Update	KB2984972
Update	KB2836502	Update	KB2888049	Security Update	KB2984977
Update	KB2836942	Update	KB2891804	Update	KB2985461
Update	KB2836943	Security Update	KB2892074	Security Update	KB2987107
Security Update	KB2839894	Security Update	KB2893294	Security Update	KB2991963
Security Update	KB2840149	Update	KB2893519	Security Update	KB2992611
Security Update	KB2840631	Security Update	KB2893984	Update	KB2993651
Update	KB2843630	Security Update	KB2894844	Update	KB2999226
Security Update	KB2844286	Security Update	KB2898785	Security Update	KB3003743
Security Update	KB2845187	Security Update	KB2900986	Security Update	KB3004361
Update	KB2846960	Update	KB2904266	Security Update	KB3004375
Security Update	KB2847311	Update	KB2908783	Security Update	KB3005607
Security Update	KB2847927	Security Update	KB2911501	Update	KB3006121
Security Update	KB2849470	Security Update	KB2912390	Hotfix	KB3006137
Security Update	KB2850851	Update	KB2913152	Security Update	KB3006226
Update	KB2852386	Update	KB2913431	Update	KB3006625
Update	KB2853952	Security Update	KB2913602	Security Update	KB3010788
Update	KB2857650	Update	KB2918077	Security Update	KB3011780
Security Update	KB2861191	Update	KB2919469	Update	KB3013531
Security Update	KB3019215	Security Update	KB3070738	Security Update	KB3134214
Update	KB3020338	Security Update	KB3071756	Update	KB3135445
Update	KB3020369	Security Update	KB3072630	Update	KB3137061
Update	KB3020370	Security Update	KB3072633	Update	KB3138378
Security Update	KB3020388	Security Update	KB3074886	Update	KB3138612
Security Update	KB3021674	Security Update	KB3075226	Security Update	KB3138910
Update	KB3021917	Update	KB3075249	Security Update	KB3139398
Security Update	KB3022777	Security Update	KB3075516	Security Update	KB3139914
Security Update	KB3023215	Security Update	KB3076895	Update	KB3140245
Security Update	KB3030377	Security Update	KB3076949	Update	KB3147071
Security Update	KB3031432	Security Update	KB3078601	Security Update	KB3155178
Security Update	KB3032655	Update	KB3078667	Security Update	KB3156016
Security Update	KB3033889	Security Update	KB3079904	Security Update	KB3156019
Security Update	KB3033929	Update	KB3080079	Security Update	KB3159398
Security Update	KB3035126	Update	KB3080149	Update	KB3161102
Security Update	KB3035132	Security Update	KB3080446	Security Update	KB3161949
Security Update	KB3037574	Security Update	KB3084135	Security Update	KB3161958

Security Update	KB3039066	Security Update	KB3086255	Security Update	KB3170455
Update	KB3040272	Security Update	KB3087039	Update	KB3170735
Security Update	KB3042058	Security Update	KB3092601	Update	KB3172605
Security Update	KB3042553	Update	KB3092627	Update	KB3179573
Security Update	KB3045171	Security Update	KB3093513	Update	KB3181988
Security Update	KB3045685	Security Update	KB3097966	Update	KB3184143
Security Update	KB3045999	Security Update	KB3101722	Update	KB4014504
Security Update	KB3046002	Update	KB3102429	Update	KB958488
Security Update	KB3046017	Update	KB3107998	Update	KB977002
Security Update	KB3046269	Security Update	KB3108371	Update	KB977902
Security Update	KB3046482	Security Update	KB3108381	Update	KB982018
Security Update	KB3048070	Security Update	KB3108664	Security Update	KB4019264
Update	KB3054476	Security Update	KB3108670	Security Update	KB3069392
Security Update	KB3055642	Security Update	KB3109094	Security Update	KB3069772
Security Update	KB3057154	Security Update	KB3109103	Security Update	KB3070102
Security Update	KB3059317	Security Update	KB3109560	Security Update	KB3126587
Security Update	KB3060716	Security Update	KB3110329	Security Update	KB3126593
Security Update	KB3061518	Update	KB3112148	Update	KB3133977
Security Update	KB3063858	Security Update	KB3115858	Security Update	KB3067903
Security Update	KB3065822	Update	KB3121255	Update	KB3068708
Update	KB3065979	Security Update	KB3123479	Security Update	KB3124280
Security Update	KB3067505	Security Update	KB3124001	Security Update	KB3126446

Windows 10 Enterprise LTSB 1607

Update	KB4345418
Update	KB4033393
Update	KB4049411
Update	KB4033631
Update	KB4132216

Antivirus

Symantec Endpoint Protection Version 14 (14.0 RU1 MP1) build 3897 (14.0.3897.1101) anti-virus software is supported. It is recommended that Network Threat Protection is disabled on the Acquisition PC.

Agilent 7890 GC Support

Supported Hardware Configurations

Agilent 7890 GC system

PTV, COC, Split/Splitless, Purged Packed Volatile Interface and Multimode inlets.

Agilent 7683B Autosampler

Agilent 7693A Autosampler

GC PAL and Combi PAL Autosampler

Agilent 7890GC Dean Switch and 2-way splitter by EPC

Agilent 7890 GC detectors supported are:

- Flame Ionization Detector (FID)
- Thermal Conductivity Detector (TCD)
- Micro-Electron Capture Detector (micro-ECD)

Other options:

PCM control of Dean Switch via GC panel only

Gerstel CIS-4 injector pneumatic control only.

Fault Fixes

Agilent 7890 – PTV can now ramped up to 720^{o}C

Agilent 7890 – accuracy is increased to 3 decimal points for the initial column flow.

Notes and concessions

1. Any new inlet file **must** be based either on the default inlet file, or on another inlet file that itself is based on the default inlet file. Otherwise the method may not download successfully.
2. The default inlet file, **default.a7890, must not be deleted from the system.**
3. If any changes are made to the default.a7890 file then it is recommended that the changes are saved with a different file name.
4. If a new MassLynx project is created, it must be based on the default MassLynx project (or on another MassLynx project that is itself based on the default MassLynx project). If not, any necessary files (e.g. default.a7890, CTC autosampler macros) must be manually copied into the new MassLynx project.
5. The A7890 method editor can be used to edit existing A7890 methods or to create new A7890 methods. The A7890 method editor can be invoked from inlets buttons (Pump, Autosampler or Detector button) available on the left side of the Inlet Method Editor.
6. To print an A7890 method, the A7890 method file must be opened once in the A7890 method editor.
7. Sampler offset must not be activated in dual injection tower mode. Otherwise the autosampler parameters will not download.
8. The ‘Allow Sampling Offset’ option available in the Front/Back Injector tab of the A7890 method editor does not work as expected. Even when the sample offset option is disabled in the A7890 method editor, a static value of ‘10mm’ is downloaded to the instrument. If the sample offset is not required to be used in routine sample analysis then the ‘Allow Sample Offset’ option should be enabled in the method editor and should be set to value ‘0.0mm’. This will ensure that the offset option is switched off on the instrument.

9. AutoPrep functionality is not supported with MassLynx.
10. To stop the current inlet method, the run must be manually stopped from the GC instrument front panel. However, when using a GC PAL, do not stop the method until after the 'Running' LED has changed to green, otherwise the next sample will go straight to Acquire and the inlet method will not be run. The 'Running' LED is on the inlet method editor.
11. To control a GC PAL or Combi PAL with the 7890 GC, the PAL must be configured with an 'Out' signal called Prep.
12. The sample list may randomly stop with 'Waiting for Prep Run' status when using a CTC PAL. The inlet method is not run, and there is no error message. The sample batch can be restarted by pressing Prep on the GC.

The workaround is to increase the length of the Pulse Times for the Prep signal on the PAL to 500 ms. The Pulse Times for CTC PAL can be set on CTC PAL instrument control panel through: 'Setup/Objects/Out Signals/Prep' menu.

13. If a FID, TCD or micro-ECD detector is connected on the A7890 GC instrument and data is to be acquired from the detector, the detector must be configured as 'A7890' from the Inlet Method editor ->Tools -> Instrument Configuration menu option.

When the detector is configured, the 'Channel 1' or 'Channel 2' option must be enabled. Also, 'Front Detector' or 'Back Detector' must be selected as the Output channel in the 'Channel 1' tab of the A7890 method file (or 'Channel 2' tab if Channel 2 is selected). Attempting to acquire data with a detector configured but the 'Channel 1' or 'Channel 2' option disabled in the A7890 method, will result in the sample list pausing at the end of each sample with the error 'No data was acquired on detector'.

14. If a FID, TCD or micro-ECD detector is connected on the A7890 GC instrument but there is no intention to acquire the detector data, de-configure the detector from the Inlet Method editor ->Tools -> Instrument Configuration menu option and ensure the 'Channel 1' and 'Channel 2' option is disabled in the A7890 method file.

Alternatively, the 'Channel 1' or 'Channel 2' option can be left enabled but a valid source option (such as Oven Temperature or Front Inlet Pressure etc) must be selected in the Channel 1 or Channel 2 tab accordingly.

Note that in a new A7890 method file the 'Channel 1' option is enabled and, on the 'Channel 1' page, the 'Source' field is configured to 'Front Detector Output' by default. The 'Channel 1' option' will need to be disabled or a valid source option must be selected.

15. If a FID, TCD or micro-ECD detector is not connected on the A7890 GC instrument and there is no intention to acquire the detector data, de-configure the detector from the Inlet Method editor ->Tools -> Instrument Configuration menu option and ensure the 'Channel 1' and 'Channel 2' option is disabled in the A7890 method file.
16. If the A7890 GC column is connected to the MS then ensure that the output of the column is set to **MSD** in the A7890 method. It allows the column to maintain proper backing pressure
17. If the outlet of the A7890 GC column is connected to the MS through an **APGC** interface, then ensure that the outlet of the column is set to the '**Other'** option in the A7890 method file.
18. The A7890 GC instrument supports different hardware configurations as stated in the 'Supported Hardware Configurations' section above. The parameters that are configured in the A7890 method file should match the hardware configurations that are available on the A7890 GC system. Failing to do so will cause an error in the Inlet Method editor. Selecting 'Reset Communication' from the Inlet Method tools menu will reset the error.

Installation

Please ensure that any previously installed A7890 ICS is removed before installing.

Uninstall any previous version of A7890 ICS, as follows:

1. Start Inlet Method editor.

2. Ensure that 'A7890' inlet is de-configured from 'Instrument Configuration' wizard.
3. Close Inlet Method editor and MassLynx.
4. Invoke Windows Control Panel's 'Programs and Features' option from <Start><Settings> <Control Panel> option.
5. Search for 'Waters A7890 ICS software' from the installed programs list.
6. Click on the 'Change/Remove' available against the program. A7890 ICS un-installation set up program starts up.
7. Follow through the instructions of the set up program to complete uninstall process.

Please ensure that only SCN 977 is installed. If any other SCN besides SCN 977 is installed then it must be uninstalled first.

Agilent 7890 GC Firmware version V A.01.10.1 was validated with this SCN. This must be the minimum version required for the support of the Agilent 7890 GC with MassLynx.

1. Launch MassLynx.
2. Start Inlet Method editor.
3. Invoke 'Inlet Configuration' dialog from Inlet Method->Tools->Instrument Configuration option.
4. Use the "Setup Instrument" button from the Inlet Configuration wizard to launch the Agilent 7890 ICS installation.
5. Once the ICS installation is completed; configure the A7890 in the Inlet Configuration wizard.
6. Close MassLynx.
7. If using one LAN card and a hub go to step 8. If using two LAN cards instead of a hub, follow the steps below.
    i. Make a note of the IP address of the A7890 GC instrument connected to the host PC. The IP address of the instrument is available on the A7890 instrument control panel. Use <Options> key and scroll to the "Communications" section and press <Enter>. The IP address should be in the form of 192.168.000.xxx.
    ii. Launch Control Panel from the Windows Start Menu
    iii. Double click on the 'Network Connections' application listed in Control Panel
    iv. In the 'Network Settings' window right click on the Ethernet device connected to the GC instrument and select the 'Properties' option. The LAN properties dialog pops up.
    v. Select 'Internet Protocol (TCP/IP)' option on the LAN properties dialog and click on the 'Properties' button. 'Internet Protocol (TCP/IP) Properties' dialog pops up
    vi. Ensure that the IP address and sub-net mask on the ''Internet Protocol (TCP/IP) Properties' dialog are set as defined below:
        a) Select 'Use the following IP address'.
        b) Set the IP Address: 192.168.000.xxx (Doesn't have to be specifically this value, but must not be the same as the IP address of the GC instrument). The IP address of the GC instrument was obtained in step 13(i).
        c) Set up Subnet mask: 255.255.255.000
    vii. Click on 'Ok' button to close 'Internet Protocol (TCP/IP) Properties' dialog.
    viii. Click on the 'OK' button on the LAN Properties window to complete the LAN configuration set up.

ix. Go to step 8.

8. Configure the Waters DHCP for the A7890 as shown in the steps below.
   i. Ensure MassLynx is closed.
   ii. Ensure that A7890 GC instrument is connected to host PC.
   iii. Make a note of the GC IP address, MAC address and serial number of the A7890 GC instrument connected to the host PC. These details can be obtained as follows:-
      a) The IP address and MAC address of the instrument are available on the A7890 instrument control panel. Use <Options> key and scroll to the "Communications" section and press <Enter>. The IP address should be in the form of 192.168.000.xxx and the MAC address should be in the form of 00-XX-XX-XX-XX-XX.
      b) A7890 instrument serial number is seen on the bottom left of the instrument front body panel. (Below the control panel).
   iv. Run 'C:\Program Files (x86)\Waters Instruments\ Waters DHCP Server Configuration.exe'. Waters DHCP Server configuration window pops up.
   v. Click on 'Add' button to add a new DHCP entry for A7890 instrument. The 'Add IP Address' dialog pops up.
   vi. Update the 'Add IP Address' dialog with the below details:
      a) Update the 'IP Address' and 'MAC Address' fields with the corresponding values noted in Step 14(iii).
      b) Select the 'Instrument Type' as 'A7890' from drop down option.
      c) Enter the serial number noted in Step 14(iii) into the 'Serial Number/Unique Name' field.
   vii. Click on 'OK' button to complete the Waters DHCP configuration for A7890 GC instrument.

From the Inlet Method Editor, reset the GC communication.