

Title: SELECT SERIES MRT Software Release 7.2

Document No: 721028084

Version No: 03

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Introduction:

Waters Embedded Analyser Platform 2.7.2 is the Release 7 installer for instrument control of the SELECT SERIES MRT Instrument

MassLynx SCN1026- Release 6 is installer of the Data System for SELECT SERIES MRT Instrument

Waters Embedded Analyser Platform 2.7.2 is for use only with versions of MassLynx SCN1026 Build Release 6 or above

No LC /Inlet driver is included with this release. SELECT SERIES instruments are supported by LC Driver Pack releases from 2019 DP1 onwards.

A Standalone LC Driver is available for μ BSM control for DESI solvents

The release is exclusively for the SELECT SERIES MRT instrument.

Included Drivers:

IMPORTANT: Waters Embedded Analyser Platform for MRT Release 7 and supporting software is only to be deployed by an Engineer trained in the Installation of SELECT SERIES MRT Software

MS Driver	Version
Waters Embedded Analyser Platform for MRT	Release 7
Data System	Version
MassLynx SCN1026	Release 6

Supported LC Driver Packs:

LC/ Inlets	Version
Waters Driver Pack 2022 Release 1	667006778RevA - Microscale

Supported Components:

The Waters Embedded Analyser Platform Release 7 installation supports the following source types:

ESI Lockspray

APci Lockspray

ASAP

Nano Lockspray

DESI

DESI-XS

DESI-XS with Heated Transfer Line

MALDI

MALDI Set Up

Operating Systems:

Waters Embedded Analyser Platform for MRT Release 7 and MassLynx SCN1026- Release 6 is supported on English version of Microsoft® Windows® 10 Enterprise LTSC 1809 on a Waters supplied DELL Precision 5820 or 5860XL and and Windows® 11 Enterprise LTSC 2024 on a Waters supplied DELL Precision 5860XL. For up-to-date information please refer to <https://help.waters.com/help/en/product-support/waters-connect-software-solutions-support/informatics-hardware-documentation.html>

Security:

Security is not supported.

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Installation:

Installation is to be carried out only by Waters trained engineers

Installation of Stand-Alone Applications:

HDI V1.6 or above with a modified version of MaldiChrom to improve processing performance with high resolution data.

Waters Embedded Analyser Platform for MRT Release 7

New Features, Enhancements and Addressed Issues:

The following table contains a list of software enhancements and addressed issues included in Waters Embedded Analyser Platform for SELECT SERIES MRT Release 7

Item	Description
(AMS-8923) - Software control for Resolution Enhancement Mode (REM) is enabled when the hardware option is detected introduced	REM extends the flight path by deflecting ions back for a second pass of the MRT analyser increasing the resolving power by >50% enabling >300,000 FWHM.
(AMS-8720) - Ability for methods to acquire data at 20Hz and 30Hz introduced	The ability to run at 20Hz and 30Hz in method acquisitions has now been introduced.
(AMS-6738) - Imaging - Auto Apply corrections from intensity preview to motion parameters feature introduced	When the imaging intensity preview is manually aligned to the sample, the adjustment can now be auto applied to the motion parameters.
(AMS-6909) - Imaging MALDI - Well Plate external Lockmass functionality feature introduced	A lockmass well can now be specified in MALDI imaging methods.
(AMS-8015) - Method editor Function number colour feature improvements introduced	Function number colour in method editor was difficult to identify. The font colour was changed to improve readability.
(AMS-8307) - Method editor mass range for MRT and Diamond mode free form test entry feature introduced	The mass range definition for MRT and Diamond mode are now free text entry if defaults are not required, allowing a user defined mass range between 20 and 2400 / 9600 m/z.
(AMS-8320) - CLMC parameters for non imaging methods with lockmass auto update feature introduced	When a non imaging method with lockmass is now created, the CLMC parameters are defined from the lockmass parameters to ensure synchronisation.
(AMS-8512) - Imaging Tune pages full size opening feature introduced	Imaging tune pages now open to full screen size when deployed from the main tune page.
(AMS - 8624) - DRE implemented for end user feature introduced	There is now a DRE control present in the Quartz tune page, the DRE control allows attenuation of the signal within the MRT.
(AMS-8631) - Tune page Timer refactor introduced	Tune page timer updated to have three digits for hours rather than the 2 digits for 'days'.
(AMS-8929) - Method editor start mass 20 m/z boundary introduced	Method editor start mass can now be set to 20 m/z, default mass remains at 50 m/z.
(AMS-6691) - DESI - Stage requires power recycle after lid is opened/closed issue resolved	Implemented a control to 'reset' the stage on the imaging UI which re-enables use and mitigates the requirement for a power recycle.
(AMS-7942) - Tune page acquired Data not selected for calibration use appears in the manual calibration list issue resolved	When data is acquired from the tune page, and the 'Retain data for mass calibration' box is not selected, the data will now not appear in the manual calibration drop down list ensuring correct behaviour.

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(AMS-8128) - Data view pop out TIC behaviour issue resolved	When the TIC is viewed in a pop out data viewer window, if then changed to BPI view, it was still showing a TIC value. This issue is now resolved.
(AMS-8221) - MALDI - Source Load/Unload control text missing issue resolved	Subtext in the MALDI load/unload update box was missing. this is now resolved.
(AMS-8300) - Desolvation heater health check issue resolved	The desolvation heater health check was not activating when the temperature value was incorrect (for example in an instance of the desolvation heater failing). This is now resolved.
(AMS-8507) - Tune page Spectrum Zoom function issue	If a range was selected for zoom on the tune page, the view was snapping to the end of the range and not displaying the full range. This issue is now resolved.
(AMS-8439) – MALDI 384 well plate only acquires to region 256 then reverts to sample 1	MALDI 384 well plate methods now run and acquire as expected. Issue Resolved

MassLynx SELECT SERIES MRT SCN1026 Release 6

New Features, Enhancements and Addressed Issues:

The following table contains a list of software enhancements and addressed issues included in MassLynx SELECT SERIES MRT SCN1026 Release 6

Enhancements introduced and issues resolved	
(AMS-8321) – Isotope model to generate theoretical continuum data feature introduced	Isotope model in MassLynx updated so that representation of MRT data can now be achieved with regards to theoretical continuum data and reference to the elemental formula isotopic range.

Concessions:

With relation to Waters Embedded Analyser Platform for MRT Release 7 the following table contains a list of characterized software issues and where available temporary work arounds and usability advice.

Known software issues	
Item	Description
(AMS-6220) – XIC initial view Y axis label can be incorrect	If an extracted mass chromatogram is opened from the Tune Page Plot view (CTRL+SHIFT and right drag across mass range of interest on the Tune Page Plot view), the label for the Y axis is not displayed correctly. This does not affect functionality.
(AMS-8947) - Intermittent loss of beam if left in REM mode for a long period when not acquiring.	If the instrument is left in REM mode for long periods of time, occasionally the ion beam signal is lost. If observed, a polarity switch will recover with no EPC reboots required.
(AMS-7404) - DESI - Sample list issue if method aborted between rows that affects the trigger signal	If a DESI method is run from the sample list, and the sample list is stopped via the ML control before the sprayer position reaches the required selected area, the sample list behaves as if it is still active though in a paused state. This also means that you cannot restart a new method (even if the process is deleted from the queue). To release the sample list, you have to delete the folder created for the aborted run (current MassLynx project/Data folder/name of folder that was aborted) and then close and reopen ML to reset typhoon

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(AMS-8780) - Incorrect mass resolution values stored in metadata can affect third party processing	Incorrect resolution is occasionally calculated and added to the extern.inf. Very high values are populated. This does not affect Waters processing but can have an impact on third party processing applications. Manually setting the Resolution value in the extern.inf file will allow correct processing (current MassLynx project/Data folder/name of sample folder required\extern.inf).
(AMS-8439) - MALDI 384 well plate doesn't acquire past sample 256	At present, do not run past well 256 in a sample list.
(AMS-8922) - Tune page report spectrum window is not fully visible	When a tune page report is printed, the Spectrum section is out of the margins.
(AMS-8771) - Method editor collision energy flat ramp causes the method to hang	If an MSMS or MSe method has a flat ramp for Collision Energy, then the method will not run. For instance, if the CE ramp is 7V to 7V, then it will not run. if 7V-8V then it will run. Recommend use of a fixed collision energy but if a ramp is used there has to be a delta between the start and end voltage.
(AMS-9012) - Typhoon Services do not always close from the MassLynx Reset Instrument control	On occasion, using the reset instrument from the MassLynx side menu gives a warning that typhoon services cannot be closed. Closing and reopening MassLynx will then fully stop/start the services as expected.
(AMS-9026) - Tune page crashes when overwriting a datafile that is open in MassLynx	When acquiring from the tune page, do not attempt to overwrite an existing data file if it is open in MassLynx Chromatogram or Spectrum windows. If data must be overwritten after it has been visualised in Chromatogram or Spectrum, it should be deleted from within MassLynx select File>open from with Chromatogram or Spectrum and then highlight the data file and press Delete. The data can now be overwritten from the tune page. This does not affect data files acquired from the MassLynx sample list.
(AMS-9036) - MassLynx Inlet shutdown is not triggered by MRT health check errors.	When a health check error is triggered and Masslynx shutdown is configured to act upon MS error, the shutdown method should run, currently it does not. This can result in wasted solvent.
(AMS-9098) – Occasional loss of beam if left in operate but not acquiring	On occasion, especially if the instrument has been left idle for long periods but in operate, the beam can appear to be lost. Switch instrument to standby. Select opposite polarity and switch to operate. Switch again to standby and back to the desired polarity, switch to operate.

Informational:

Opening MassLynx will start the instrument control services. Closing MassLynx will stop the instrument control Services.
Prior to running manual Instrument set up routines, the user should ensure that the calibrant peaks of interest are optimal.
Tune Sets for sample optimisation can be loaded, if further modified they will be denoted with an Asterisk until a further save is carried out. Tune sets will require re-loading post instrument reset.

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Detector Set up can be run using an ESI source or MALDI Setup Source utilizing a syringe drive or other solvent delivery pump loaded with the applicable specified sample (Leucine enkephalin).
Calibrations can be applied using a MALDI, DESI or ESI Source utilizing an applicable sample from the manual calibration page.
Do NOT switch off or reboot the instrument to disconnect/reconnect the DESI source or instrument set up routines will be invalidated and require a re-run.
If a tune set is to be added to the MassLynx sample list 'MS Tune File', Manual navigation to the following location is required to select the required tune set C:\Waters Corporation\Typhoon\run\tunesets. This will need to be repeated for each desired file or they can be manually modified in the MS Tune File text box.
Ensure the instrument is set to Standby (not Source Standby) before switching polarity. When 'Operate' is used, Tune or Abort will be disabled until the detector reaches working voltage.
Source pressure test not required if a DESI Source is fitted.
When a Health Check is present for the Push, Pull or Pull2 Voltages (check the Health Status page if no beam is present when in Tune), please contact the AMST Test and Install Group to resolve the issue.
Detector Set up – Optimize the beam in Diamond Mode before Running Detector set up. The application will then take over when it is running to optimize further.
If running Well plate experiments in MALDI or DESI, First configure the sample list to show the Region ID and Well ID Columns (right click and 'Customize Display').
Well plate experiments require the user to create a Base method (MS, MSMS, MSe) and the use the 'Export' control at the top of the source control page to make the selection of the well positions required. Once saved, this can then be populated on the sample list using the MassLynx File>Import Worksheet control. Each time you use this control the previous sample list view will change to the new Worksheet. With current implementation you cannot 'merge' multiple worksheets into a single sample list.
With current implementation, if you try to Run a well plate experiment from the tune page it will run all potential wells on your configured slide. The recommendation is to run it via sample list after exporting your well selection using the tool provided
With current implementation, if values on the imaging stage control page are changed (for example scan time) for well plate methods, then it will have to be saved to the method and exported as a new worksheet for the changes to take effect. This does not affect Constant Velocity experiments from the tune page
Opening MassLynx will start the instrument control services. Closing MassLynx will stop the instrument control Services.
A hard or soft reboot of the instrument EPC will clear manual instrument set up Calibrations only. They will be required to be re-run to ensure correct operation
When switching to REM, The tune button will disable for several seconds as voltages settle. Same will be observed when switching from REM. If running from a sample list and tune page is in a different mode, then the list will halt momentarily to accommodate the voltage switch before resuming.
DESI - If after the source door has been opened and closed there is no stage movement, use the 'Reset' control in the DESI status pane to reinitialize.
For optimum mass accuracy the user is advised to allow >5 minutes of settle time after switching to REM before acquiring data. The same time duration should be applied when initially acquiring data for manual calibration.
When acquiring a mixed mode sample list (MRT / REM) optimum mass accuracy will be achieved if a blank injection(s) is performed after switching modes to allow for a >5 minutes settle.

In REM, highest mass accuracy is achieved when the m/z of interest is within the m/z range of the calibration profile.
REM - when configuring a lockmass for the discrete ranges, ensure the lockmass peak of interest is within the range being acquired
If navigation away from and then back to REM, the mass range will default to 50-150m/z range. It requires you to select the correct range for your analyte after this sequence.
In REM, space charge effects within the analyser can lead to decreases in m/z resolution and may be observed for peak areas >2e6 at 1 Hz, the effect may be more prominent for multiply charged ions
MALDI - Laser repetition rate should not be set to a value over 2500Hz
MALDI - Load and unload is now a single control which carries out the venting/pumping and opening /closing of the valve

Supported Computers, Operating systems, Hotfixes and Anti-Virus software:

For up-to-date information on Waters SELECT SERIES MRT supported computer and operating system please refer to <https://help.waters.com/help/en/product-support/waters-connect-software-solutions-support/informatics-hardware-documentation.html>

Windows updates should be disabled through the Microsoft System Configuration – Services tool.

The PC firewall can occasionally be re-enabled by windows updates. After every update the firewall must be checked to ensure it is still disabled or correct exceptions applied.

The use of Endpoint Protection/Security (AV, Domain and Firewalls) is not recommended.

Where company policy dictates the use of Endpoint Protection, correct exceptions **must** be applied that is applicable to the variant of protection installed.

Failure to apply the exceptions is known to induce Communication Failures between Hardware and software which can manifest as erroneous behaviour of instrument control and data system.

Waters strongly advise customers to request help from their IT support to ensure the Endpoint Protection environment is configured appropriately.

If additional advice and assistance is required, please contact a Waters service representative.

Remote Desktop Connection with MassLynx 4.2 is not advised and is known to cause communication issues between the Hardware and Software which can result in a reset of the instrument and PC being required.

If additional advice and assistance is required, please contact a Waters service representative.

The following Windows Updates (Hotfixes) are supported with MassLynx V4.2 SCN1026 Release 6 and Waters Embedded Analyser Platform Release 7:

Update	KB5005540		Update	KB4589208
Update	KB4470788		Update	KB5005112
Update	KB4486153		Update	KB5007206
Update	KB4487038		Update	KB5006754
Update	KB4535680		Update	KB 5005701
Update	KB4577586			