HDI 1.7

Release Notes

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HDI 1.7 3
INTRODUCTION 3
APPLIES TO 3
OPERATING SYSTEMS 3
SECURITY 4
INSTALLATION PROCEDURE 4
UNINSTALLATION 5
APPLICATIONS 5
ENHANCEMENTS 5
FAULT FIXES 6
CONCESSIONS 7
INFORMATIONAL 7
HARDWARE NOTES 7
GPU COMPUTING CARD SETUP 8
HOTFIXES 8
ANTIVIRUS 10
WINDOWS UPDATES 10

HDI 1.7

Introduction

HDI v1.7 supersedes HDI v1.6. This software introduces support for the Xevo TQ Absolute instrument DESI XS HTL source and integration of DESI Method Editor (v2.0) as a Plug-in.

It adds support for Xevo G3 QToF, MRT mass spectrometer DESI data, and HDI general improvements for existing instruments.

HDI v1.7 includes enhancements, fault fixes, and concessions as described in the Enhancements, Fault fixes, and Concessions sections of this document.

Applies to

- Xevo G3-XS with DESI source
- SYNAPT XS with DESI and/or MALDI sources
- Xevo TQ Absolute with DESI source
- Xevo G2-XS with DESI source
- MRT with DESI and/or MALDI sources (MS and MSMS)
- Cyclic IMS with a DESI source for IMS (HDMS only) mode

Note: MALDI SYNAPT, MALDI SYNAPT G2, and MALDI SYNAPT G2-S are not supported by this release.

Operating systems

Supported PC	Supported operating system
Lenovo P520	• Microsoft® Windows® 10 Enterprise LTSC 2021 (64-bit) • Microsoft Windows 10 Enterprise LTSB 1607 (64-bit)
Lenovo P720	• Microsoft Windows 10 Enterprise LTSB 1607 (64-bit) • Microsoft Windows 10 Enterprise LTSC 2021 (64-bit)

Note: Xevo TQ Absolute is tested and supported on P520 only.

Security

MassLynx security is not supported.

Installation procedure

HDI v1.7 is a complete installation. If an earlier version of HDI is already installed, it must be uninstalled before installation of HDI 1.7.

Note: To remove HDI completely, you must delete the 'C:\HDI' folder following removal of the software. In the case of an upgrade from a previous version to HDI 1.7, you must delete the existing 'C:\HDI' and 'C:\HDImaging' folders following removal of the software.

This is vital when uninstalling one version of HDI in order to reinstall an older version.

Note: Before HDI v1.7 is installed, existing installations of DESI Method Editor should be uninstalled using Add/Remove Programs.

Prerequisites:

- It is assumed that an appropriate MassLynx 4.2 (Instrument Control) for a supported Xevo TQ Absolute or Xevo/SYNAPT series instrument is already installed on the machine before HDI is installed.
- Ensure that the key disk is available before installation.

Note: This procedure requires Windows Administrator privileges, and the user must logon to the computer as a local administrator (not any other/domain user with local administrator rights).

1. Insert the HDI v1.7 media into the drive.
2. Double-click the setup.exe file in the root folder.
3. Click **Next**.
4. Select **I accept the terms in license agreement**.
5. Click **Next**.
6. For Xevo TQ Absolute instrument, select **Triple Quad(TQ)**.
    a. Click **Next**
    b. Click **Install**.
    c. Click **Browse** and locate the HDI keydisk drive.
    d. Click **OK**.
    e. Click **Continue** to complete the installation.
    f. Select **Finish**.

Note: If you do not have keydisk, contact your MassLynx system administrator.

Note: The Acquire tab is not visible for a Xevo TQ Absolute instrument.

Note: You have the option to clear the selection of WatersRawAnalyze7.5Convertor.

7. For high resolution TOF, select **High resolution TOF**.

Note: Depending on the option selected for WatersRaw7.5Converter, the applications will be installed. If installed, a desktop icon is added.

Note: Keydisk is not required.

Note: The Acquire tab is visible for a high-resolution TOF instrument.

a. Click **Next**.

b. Click **Install**.

c. Click **Finish**. The HDI v1.7 shortcut is added to the desktop.

Note: The Desi Method Editor can be launched by opening the HDI > Plugins tab.

Note: WatersRaw7.5Converter is optional.

8. Launch HDI v1.7 from the item on the Start menu or the desktop shortcut.

Uninstallation

HDI v1.7 can be removed by using the Programs and Features option in the Windows Control Panel.

Note: For a TQ instrument, uninstalling HDI also uninstalls DESI Method Editor.

APPLICATIONS

Enhancements

The following are the software enhancements included in HDI v1.7.

- HDI can handle files up to 20 GB. It can process and analyze the high-resolution data acquired on instruments with increased sensitivity.
- To improve processing time, all scans combined into a single spectrum are stored in raw data and referred to in subsequent requests for additional processing.
- Updated installer for selection of instrument, with the available options of Xevo TQ Absolute or a High Resolution (TOF) instrument.
- The Acquire tab is available when you install HDI by selecting High resolution/TOF instrument. With Xevo TQ Absolute there is no Acquire tab. Acquisition of Xevo TQ Absolute data is defined in Plugins > Desi Method Editor.

- An integrated DESI TQ Method Editor, part of the targeted MS Imaging solution, to define MRM, SIR, MS, and MS/MS DESI imaging experiments in a sample workflow. See the DESI TQ Method Editor Help.
- Updated installer for selection of the DESI TQ Method Editor license (keydisk) as part of the targeted MS Imaging solution.
- Support for Xevo TQ Absolute allows Xevo TQ Absolute Full Scan MS and MSMS data processing on the Process tab. Load Xevo TQ Absolute MRM, SIR, Full scan MS, and MSMS data with Precursor-Product Ion representation for Xevo TQ Absolute MRM data on the Analysis tab.
- imzML converter support for Xevo TQ Absolute data.
- imzMLConverter upgraded to 0.7 version for SHA updates and updates to definitions for imzML.
- Support for MRT data.
- Support for Xevo G3 QTOF DESI data.
- Addition of Continuous LockMass Correction (CLMC) on the Process tab to correct the internal lockmass and create a lockmass corrected continuum raw data file for TOF data only (does not support IMS data format).
- TIC information appended to the Analyte file on processing in HDI, the exceptions being MRM and SIR data from Xevo TQ Absolute.
- Precursor-Product Ion representation on the Analysis tab for Xevo TQ Absolute MRM data.
- Export MVA with or without TIC normalization.
- Provision of scientific notation for intensity values on the Analysis tab.
- Save regions of interest (ROIs) from the Analysis tab and reload them.
- Use saved ROIs as processing masks on the Process tab.
- Export ROIs multi spectrum for non-mobility and mobility data.
- New spectrum plots for average intensity and sum intensity.
- WatersRawConverter renamed to WatersRawAnalyze7.5Converter. A new desktop icon is added.
- An additional wizard page is added to the HDI installer to allow WatersRawAnalyze 7.5Converter installation, making it an optional choice.

Fault fixes

The following are the faults fixed in HDI 1.7.

- Configuration file is not updated with changed parameter values if parameters are set before adding the raw data on the Processing tab.
- Disable the Internal Lockmass option for MRT MS and MRT MS/MS data.

- User is able to MVA export ROIs that are not committed.
- Peak table list values are not saved for an analyte file with 12 or fewer intense peaks.
- Spectral chart range bar for max intensity does not filter data after TIC/BPI normalization.
- “TIC normalization” is not true TIC normalization, only normalization to picked peaks. For it to be true TIC normalization, it would have to be added as a processing option, not be part of the Analysis tab.

Concessions

The following are known software issues and workarounds for HDI 1.7.

- The "build data target list" process is malfunctioning. Unless there is some text under the "header" (equating to text in the top-left corner of the analyte file when opened in Excel), the build data target list function does not work.
- HDI v1.7 can export data to .csv files. The file name for the exported file is based on the raw data in the HDI analysis, the image files used, the pattern files used, and other factors. As a result, the file name for the exported file can be long.
- When creating composite images while having a visual ROI mask applied, each time you add another ion to the composite image it resets the max intensity to 0, giving the black color. The max intensity value must be re-entered.
- When the Sample List is imported into MassLynx, it (including the File Name or the Methods) should not be changed, because that causes the linked image processing to fail.

Informational

- By default, HDI v1.7 installs files in the location C:\HDI.
- The WatersRawAnalyze7.5Convertor executable is stored at C:\HDI\bin.
- Neither SIMCA nor EZinfo software is supplied with this software. EZinfo software can be purchased separately from Waters.
- The R menu on the Spectral chart is not available with multiple data layer selection. R processing on multiple data layers is not allowed.

Hardware notes

HDI can be run on any resolution, but it is recommended that you use a high-resolution screen with minimal settings of 1920 x 1080-pixel resolution for better images.

PC setting - In Windows Control Panel, navigate to Region and Language, and select the Format tab. If the Format is not English (United Kingdom) or English (United States), select the Additional Settings option and ensure that the Decimal Symbol is a period.

GPU computing card setup

For optimum performance when analysing HDMSe, it is recommended that HDI 1.7 is installed on a PC containing a Quadro P5000/RTX 5000 NVIDIA GPU computing card.

Note: Lenovo P720 includes a GPU card.

This section describes how to set up a GPU computing card for use in HDI 1.7.

If a GPU computing card is not installed, begin at step 1. If the card is pre-installed, go to step 3.

Note: DO NOT allow Windows Update to update the drivers for the GPU and graphics cards. Doing so may result in the GPU failing to function correctly.

1. Before installing the data processing GPU card, the computer must already be set up with a graphics card to drive the display. DO NOT remove or move this card when installing the data processing GPU card because it is required to drive the display.
2. Shut down the computer, install the data processing GPU card in a PCI-Express x16 slot, and plug the power cable into the back of the data processing GPU card.
3. Disconnect any display that is connected to the data processing GPU card.
4. Download and install the latest GPU drivers from http://www.nvidia.com.

   Note. For PCs with dual NVIDIA Quadro/NVIDIA Tesla graphics cards (referred to by NVIDIA as Maximus systems), only the Quadro driver should be installed.
5. Right-click on the desktop and select “NVIDIA Control Panel” from the menu that appears.
6. Select “View System Topology” and scroll in the main window until you can see the data processing GPU.
   a. If correctly configured, Usage Mode will be TCC.
   b. Select “Change ECC State”. Ensure that the check box next to the data processing GPU is not selected. If the ECC check box is selected, clear it.

Hotfixes

HDI 1.7 was tested and validated with Lenovo P720 with Quadro P5000/RTX 5000 data processing GPU card on Windows 10 Enterprise LTSC 2021 (64-bit) and Windows 10 Enterprise LTSB 1607 (64-bit), and with Lenovo P520 (without GPU card) on Windows 10 Enterprise LTSC 2021 (64-bit) and Windows 10 Enterprise LTSB 1607 (64-bit).

The following Windows Updates are supported with HDI 1.7:

Windows 10 Updates for Lenovo P520 Microsoft Windows 10 Enterprise LTSC 2021 (64-bit)

Description	HotFix ID
Security Update	KB5020872
Security Update	KB5012170
Security Update	KB5022282
Update	KB5016705
Update	KB5018506
Update	KB5020372
Update	KB5005699
Update	KB5003791

Windows 10 Updates for Lenovo P520 Microsoft Windows 10 Enterprise LTSB 1607 (64-bit)

Description	HotFix ID
Security Update	KB5020872
Security Update	KB5012170
Security Update	KB5022282
Security Update	KB5018506
Security Update	KB5005699
Update	KB5003791
Update	KB5016705
Update	KB5020372

Windows 10 Updates for Lenovo P720 Microsoft Windows 10 Enterprise LTSC 2021 (64-bit)

Description	HotFix ID
Security Update	KB5012170

Security Update	KB5020372
Security Update	KB5022502
Security Update	KB5022834
Update	KB5003791
Update	KB5005699

Windows 10 Updates for Lenovo P720 Microsoft Windows 10 Enterprise LTSB 1607 (64-bit)

Description	HotFix ID
Security Update	KB4033631
Security Update	KB4343902
Security Update	KB5014026
Security Update	KB4493470
Feature Pack	KB4486129
Update	KB4033393
Update	KB4049411
Update	KB4132216
Update	KB4346087

Antivirus

HDI 1.7 was tested with Cortex XDR 8.0 on P520 and P720 Image with Windows 10 Enterprise LTSC 2021 (64-bit) and Windows 10 Enterprise LTSB 1607 (64-bit).

See support.waters.com for additional advice on configuring other antivirus software with Waters software.

Windows updates

The PC firewall can occasionally be re-enabled by Windows updates. After every update, check to ensure that the firewall is still disabled.