Waters[™]

High-Definition Imaging Software (HDI) 1.7 – New Features And Benefits

INTRODUCTION

Waters High-Definition Imaging (HDI) software is the heart of MS Imaging at Waters. HDI and its supporting utilities, provide the full end-to-end MS Imaging workflow for both MALDI and DESI Imaging technologies across the Waters MS Portfolio.

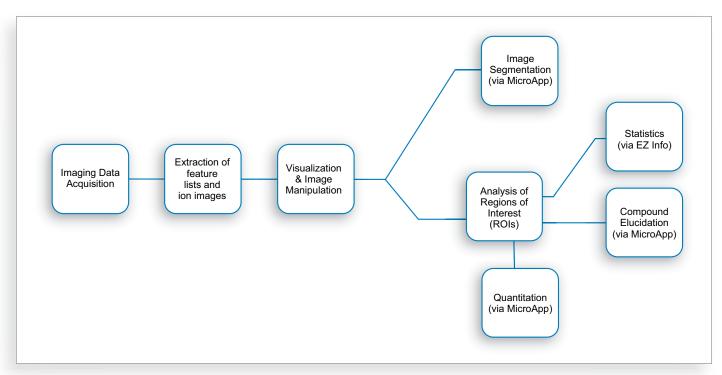
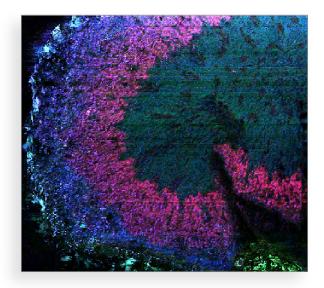


Figure 1 HDI software, in combination with MassLynx, EZ Info and MS Imaging Microapps, handles all aspects of an MSI experimental workflow from acquisition through to data analysis and interpretation of results.



HDI supports the acquisition and processing of the full range of acquisition modes including SONAR, HDMS^E, MRM, SIR, HDMS, MS, HDMS/MS and MS/MS.

The latest version, HDI 1.7, represents a significant leap forward with new features that deliver flexibility, power and speed to the analysis of MS Imaging datasets.

TARGETED WORKFLOW

For the MS imaging of known molecular species and where sensitivity and specificity are key, HDI 1.7 now supports a targeted workflow, through the acquisition and processing of MRM and SIR data sets, exclusively on the Xevo TQ Absolute. With the DESI[™] XS TQ Method Editor installed, MRM and SIR monitoring of up to 32 ions can be performed simultaneously. Ion images for scheduled functions are automatically extracted for visualization and investigation in HDI. This workflow delivers the highest specificity and sensitivity available and gives quick confident answers.

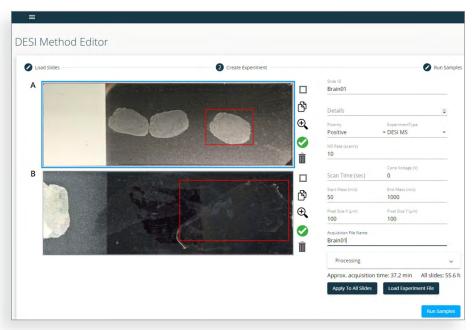


Figure 3; Targeted MS Imaging is conducted via the DESI TQ Method Editor to the core HDI software platform.

A complete quantitation workflow is now available using the MSI Quantify MicroApp. Applicable to both discovery and targeted MS Imaging data, this utility can be used to extract ROIs for standards and unknowns, plot calibration curves with appropriate statistics and use this to calculate unknown quantities in any given region of sample.

	MSI Quantify 1.0.0	Results	
Page Experiment info Add data	Make calibration curve	$y = 1.9 \cdot 10^{-7} x - 0.332$	x : summed intensity / area [µm^-2]
Add ROI Make calibration curve Evaluate	Select dose mass and normalization for calibration curve	$R^2 = 0.99324$	y : Dose [μ M]
Experiment info	267.1703 (stenolol (dilution))		
Name: spotted_liver_03Nov21	Normalization		
	None		and the second se
ROls: 9		100	•
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User guide	Select ROIs	80	
See user guske v License regulared to scill_dviske@valen.com express on 27 August, 2023			•
	809 FO3 803 803 803 803 909 909	0 100M	200M 300M 400M 500M summed intensity / area [μm^-2]

Figure 4; The MSI Quantify MicroApp makes a complete quantitation workflow possible for MS Imaging data.

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ROI SAVE, EXPORT AND REPROCESS

Regions Of Interest (ROIs) can now be saved and reloaded into the browser at a later time. This feature can not only save you time, but can also be used as a mask for data processing.

Previously it was only possible to export an ROI as a single collapsed spectra in .raw format. Now it is possible to export an ROI in .raw format as a collection of individual spectra, preserving the information contained within each individual pixel, including the drift (in IMS data) or quad (in SONAR data) dimension. The exports can then be interrogated in Masslynx or taken forward to whichever processing package you favour, such as Progenesis for a spatial omics investigation.

NEW LOCK MASS WORKFLOW

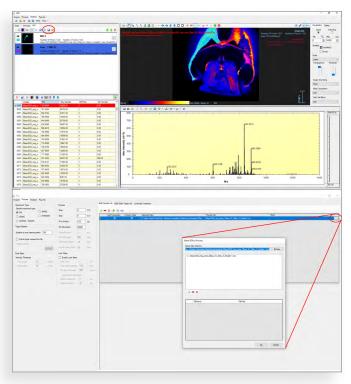


Figure 5; HDI 1.7 with flexible Region of Interest (ROI) manipulation.

HDI now has a new Continuous Lock Mass Correction (CLMC) routine that improves mass accuracy extrapolating mass shifts between lock mass calculations allowing for smoother mass adjustment.

OTHER FEATURES

- Ultimately, the combined spectrum used for peak picking is more relevant, focusing on analytes of interest from within the sample reducing the appearance of background ions from outside of the sample.
- HDI now supports the full potential of the SELECT SERIES MRT by making use of mass values to 5 decimal places.
- Spectral viewer now supports additional y-axis options including average and summed intensity as well as maximum intensity.
- imZML converter supports MRM data.



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