

Connected Solutions for Metabolomic and Lipidomic Studies on the Xevo MRT Mass Spectrometer

Make meaningful scientific discoveries more efficient through dedicated workflows combining column chemistries, separations, and informatics.



The field of metabolic and lipidomic profiling faces many challenges



The Xevo MRT Mass Spectrometer readily integrates with your existing pipeline and workflow strategy

Waters has partnered with Mass Analytica[™] and their market leading metabolomic, lipidomic and metabolite identification software packages, MARS, Lipostar2 and MassMetaSite, respectively.

Through either the waters_connect[™] Application Programming Interface (API) or via mzML*, there is the option for you to transfer your data into the relevant software package for statistical interpretation and identification of analytes.

The DATA Convert application within the waters_connect platform enables you to convert to and export mzML* file formats, ensuring a seamless integration of technology and informatics for every lab.



<u>* HUPO Proteomics Standards Initiative</u> <u># https://mzio.io/#mzmine,</u> <u>\$http://prime.psc.riken.jp/compms/msdial/main.html</u>



Flexible informatics:

Whether using a Waters supported solution or exporting data via mzML to custom scripted workflows, we have you covered.

DATA Convert

DATA Convert is embedded with the Acquisition method Editor (AME) application and automatically converts data sets into mzML format during data acquisition.

mzML is a universal file format and ensures labs can seamless integrate the Xevo MRT into their existing data pipeline.

Options are available for centroid conversion, data compression and for the export of both MS, MS/MS and DDA acquisition types.

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	Write index Includes an index to file locations of each mass spectrum and chromatogram to allow applications to quickly access required data.					
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	m/z precision Set precision for m/z ve accuracy is expected to	m/z precision Se procion m/x values in mass spectra. Selecting 64-bit will make files larger but improves precision of m/x values. This is usually only necessary where mass accuracy is expected to be better than ~1 ppm.				
-	32-bit 64-bit					
Version: 3.5.0-br-INFAME-9298-1003						

https://mass-analytica.com/products/mars/ https://mass-analytica.com/products/lipostar/

LipoStar2 — MARS

Comprehensive, vendor-neutral software for LC-MS/MS-based untargeted and semi-targeted analysis for lipidomics and metabolomics respectively, importing DDA and DIA acquisition modes.

Features Include:

- Raw data import and peak detection, identification, quantification, statistical analysis, trend analysis and biopathway analysis
- Combining of positive and negative ion mode data sets for increased knowledge and comprehensive analysis
- Fragmentation algorithms specific to the application
- Stable isotopic labelling





Factors assuring success through applications knowledge



Standard protocols for end-to-end metabolomic and lipidomic workflows with libraries to support the identification of metabolites and lipids Instrument performance and stability ideally suited for metabolic profiling Flexibility of data output and processing for easy adoption of technology Through our extensive collaboration network our scientists have the indepth knowledge and experience in omics to ensure your lab is successful

Achieve exceptional science - 100% of the time with the Xevo MRT Mass Spectrometer, a state-of-the art QTof delivering 100K resolution at 100 Hz with sub ppm mass accuracy

waters.com/XevoMRT

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