

Press Release

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European premiere: Phenomenome Profiler and MetID Solution Two new software solutions accelerate research

Exploration of differences for biomarker discovery / Identification of known and unknown metabolites

Shimadzu, one of the world leaders in analytical instrumentation, presents two new software solutions taking full benefit of the outstanding data generated by the unique hybrid mass analyzer, LCMS-IT-TOF at the Biotechnica trade exhibition in Hanover, Germany. The Phenomenome Profiler software is designed to quickly and efficiently explore differences for biomarker discovery, while the new MetID Solution software accelerates metabolite identification using a unique approach to component verification based on statistical data.

Phenomenome Profiler explores differences for biomarker discovery

Shimadzu Corporation and Phenomenome Discoveries Inc. (PDI), a leading provider of software tools for metabolomics analysis, launched enhancements to the Phenomenome Profiler™ metabolomics software to support high mass accuracy MSⁿ data. The unique mass spectrometry of the LCMS-IT-TOF quadrupole ion trap time-of-flight instrument from Shimadzu is now combined with an

integrated approach to global profiling with Phenomenome Profiler software.

The new software has been developed under an existing collaboration between the two life science companies and strengthens the integration of information-rich mass spectrometry data with the data mining tools of Phenomenome Profiler software.

Phenomenome Profiler software has been further developed to work seamlessly with the LCMS-IT-TOF technology, supporting not only high mass accuracy MSⁿ data streams, but also fast polarity switching. The new Phenomenome Profiler™ Plus software tools will help researchers view and interpret complex data sets quickly and with greater efficiency.

MetID Solution identifies known and unknown metabolites

The new MetID Solution software from Shimadzu is used for accelerating metabolite identification using high mass accuracy MSⁿ data.

The software is an integrated approach to metabolite identification which maximizes the information from data-dependent high mass accuracy MSⁿ acquisitions and accelerates effective reporting using a novel approach based on statistical data. The new platform helps researchers to find metabolites quickly using a multivariate statistical algorithm that relates parent fragment ions to predicted metabolites.

As the data is acquired using high mass accuracy and MSⁿ, the MetID Solution software searches for common ion signatures between the parent drug compound and potential metabolites. This process eliminates most of the extraneous chromatographic peaks and ions that typically complicate this type of analysis. The result is a platform that is a highly effective tool in metabolite identification and verification.

MetID Solution software has been designed with an open architecture to support not only statistics-based metabolite analysis, but also conventional peak processing routines, including mass defect, control file subtraction and user-defined biotransformation lists. In order to better visualize chemical structures and refine targeted biotransformation lists, MetID Solution can also be integrated with predictive drug metabolism software applications.

Trademarks:

Phenomenome Profiler is a registered trademark of Shimadzu and Phenomenome Discovery Inc..

MetID Solution is a registered trademark of Shimadzu.



Caption: Two new software solutions complement the high-performance mass analyzer LCMS-IT-TOF: Phenomenome Profiler software explores differences for biomarker discovery and MetID Solution software accelerates metabolite identification.

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