Waters
THE SCIENCE OF WHAT'S POSSIBLE™

METABOLYNX APPLICATION MANAGER

WATERS INFORMATICS FOR ADVANCED MS ANALYSIS

Continued innovations for small molecule profiling

Profiling small molecules in complex matrices (biological, food, or chemical) is a difficult task. Rapid detection of as many analytes as possible in the matrix, with a high degree of sensitivity and resolution, is critical. Equally important is the need for researchers to be able to easily process and interpret this large amount of data and convert it into meaningful information.

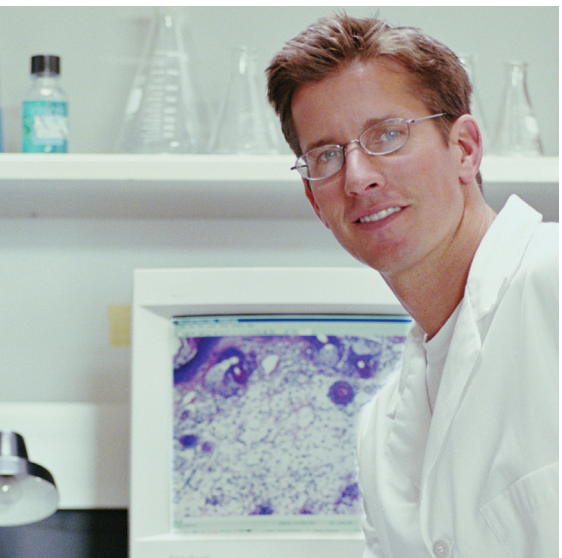
Waters has led the way in small molecule profiling with unrivalled UPLC®/MS, UPLC/HDMS™ and GC/MS system platforms along with specialized data handling and interpretation tools in MassLynx™ software to define the standard for addressing these analytical challenges.

MetaboLynx Application Manager updates for 2007

The MetaboLynx™ Application Manager for MassLynx software has been developed to aid with the detection and identification of xenobiotics for *in vitro* and *in vivo* drug metabolism studies. The software detects putative biotransformations without requiring operator-supplied predictions of metabolic fate.

The Application Manager automatically runs samples scheduled for analysis by LC/MS and processes the resulting data. Results are reported data browser that enables the chromatographic and mass spectroscopic evidence that support each automated metabolic assignment to be rapidly reviewed locally or remotely via a secure corporate network.

MetaboLynx operates by comparing and contrasting each metabolized sample with a control sample, although unexpected metabolite searching may still be performed in the absence of a suitable control. Samples from in vitro incubations or in vivo dosing experiments can be quickly analyzed by LC/MS, followed by a multi-dimensional data search that correlates retention time, m/z value, intensity, and components from alternative detection technologies (e.g. diode array UV or radiochemical monitoring). Comparison of analyte data with the control sample allows filtering of matrix-related peaks that would otherwise produce an unmanageable list of false metabolite peaks. Other essential tools such as mass defect filtering are also used to remove the generation of any possible false positives.



New MetaboLynx features:

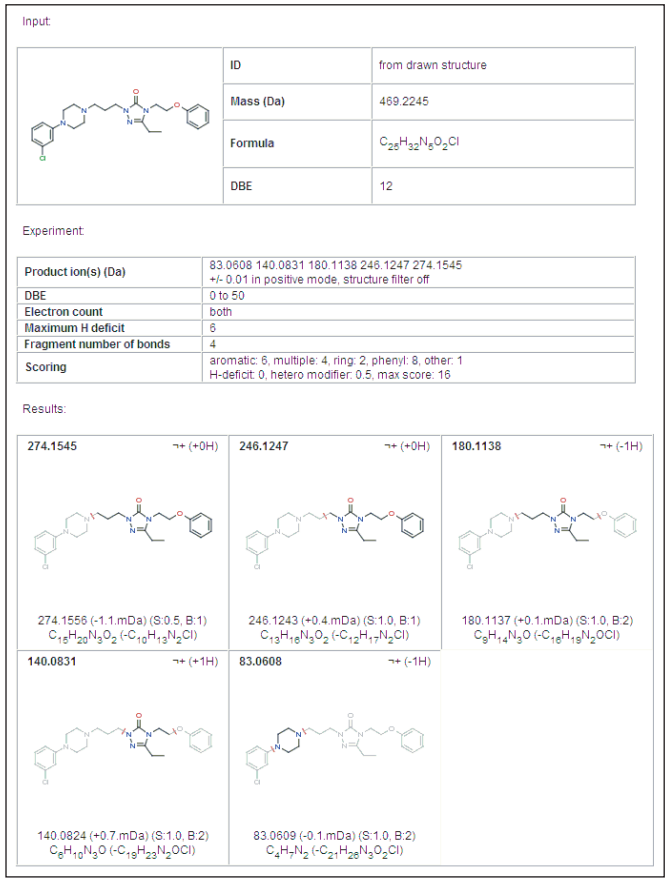
- MassFragment, a chemically intelligent structure elucidation tool
- Improved mass defect filter with the use of multiple mass ranges
- Improved MS^E data processing for fragment, precursor, and neutral loss information from a single injection

Structural elucidation

The main bottleneck in metabolite identification has also been addressed: structure elucidation. MetaboLynx provides a new approach to structure elucidation in combination with MS^E. The Triwave™ enhanced CID fragmentation data provide increased structural coverage of small molecules within a single experiment that leverage structural confirmation/elucidation studies.

MetaboLynx improves scientist's ability to study structural elucidation with MassFragment™, a chemically-intelligent structural elucidation tool developed in collaboration with scientific software experts at Dotmatics, Ltd. (Cambridge, UK). This software algorithm assigns structures by taking fragment ion spectra of the drug and/or metabolite, using it to automatically calculate fragments based on a series of novel chemically intelligent algorithms. This approach is based on systematic bond disconnection for the precursor structure instead of the traditional rule-based approach, which is limited to the extent of the rules coded and will not always provide the information required.

This important structure elucidation tool is now available to MetaboLynx users, enabling scientists to obtain faster and more informative data interpretation for expected and unexpected metabolites.



The parent drug chemically intelligent structure elucidation tool, MassFragment.

Waters

THE SCIENCE OF WHAT'S POSSIBLE.™

Waters Corporation
34 Maple Street
Milford, MA 01757 U.S.A.
T: 1 508 478 2000
F: 1 508 872 1990
www.waters.com