[MASSLYNX SOFTWARE]

Flexibility, Confidence, Efficiency

ALL IN ONE PLATFORM

Waters

THE SCIENCE OF WHAT'S POSSIBLE.®

Mass Spectrometry labs are driven by results

SAMPLE ANALYSIS IS ALL ABOUT QUESTIONS

Waters® MassLynx® Software is mass spectrometry software that answers those questions, helping your entire laboratory further advance. Productivity increases and training costs are lowered with our easy-to-use software. Run more samples faster with intelligent instrument control. Enhance confidence in your results with dedicated Application Managers that quantitate, identify, and confirm. Maintain compliance with integrated security features.

TAKE CONTROL OF MASS SPECTROMETRY ANALYSES

With today's flexible instrument configurations, sophisticated data acquisition capabilities, and detailed data processing requirements for mass spectrometry (MS) analysis, it is easy to be overwhelmed when adding or replacing legacy MS instrumentation.

In the laboratory, the challenges of MS and MS/MS analyses are often compounded by the use of several types of analytical instruments and high personnel turnover.

To maintain – and even increase – laboratory productivity, you can turn to Waters software to simplify interaction with your MS system and retain the ability to perform advanced experiments.

MassLynx improves your MS system with its intuitive interface, intelligent instrument control, and software features built around the focus of your analysis: the sample. With much of its development driven by input from our extensive user base, MassLynx has evolved into a powerful software package that reflects the versatility and flexibility you require.

Balancing simplicity and sophistication, MassLynx makes MS and MS/MS techniques available to users of any skill level, from technicians to experienced mass spectrometrists.

INSTRUMENT CONTROL WITH THE SAMPLE LIST

- Launch inlet and MS method editors.
- Run step-by-step wizards to configure and optimize your instrument system.
- Specify instrument methods for individual samples or sets of samples.
- Start, stop, and monitor the progress of your experiments.
- View the status of system components, such as the inlet and mass spectrometer.

MassLynx offers versatile control of a range of Waters Mass Spectrometers, fully integrated with a suite of ACQUITY® UPLC® and ACQUITY UPC²®® separations platforms.

DATA MANAGEMENT WITH THE SAMPLE LIST

- Enter or import sample information in a versatile spreadsheet-style format.
- Directly access spectra and chromatograms.
- Initiate automated data processing and review with OpenLynx or TargetLynx XS.
- Access advanced application-specific tools.

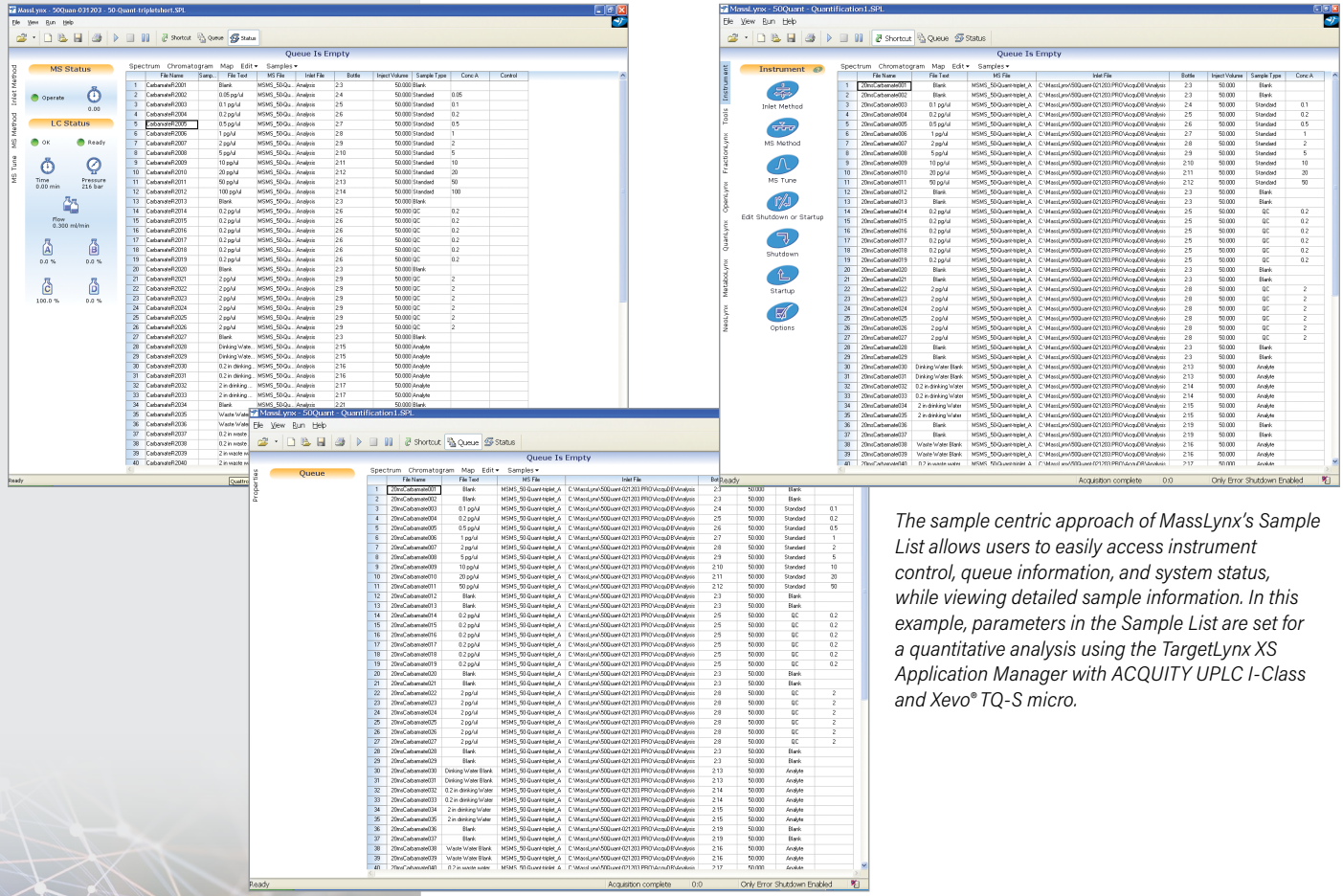
SAMPLE CENTRIC SIMPLICITY

Everything about your sample in one place

The challenge facing many laboratory analysts is not the speed of data acquisition, but the rate at which samples are converted into useful information.

MassLynx starts by giving you complete control of your analytical system within one interface: you will acquire, process data, and review results more productively than ever before. By using the individually designed and optimized data processing tools of MassLynx Application Managers, such as OpenLynx™ for processing batches of qualitative analyses and TargetLynx™ XS for quantification, samples are seamlessly converted into meaningful information – without manual data review.

At the core of MassLynx is the Sample List: the single location for initiating all activities related to your sample. By presenting all the relevant sample information in one window, MassLynx's Sample Centric™ approach simplifies your interaction with your MS system and increases the speed at which you convert samples into valuable knowledge.



The sample centric approach of MassLynx's Sample List allows users to easily access instrument control, queue information, and system status, while viewing detailed sample information. In this example, parameters in the Sample List are set for a quantitative analysis using the TargetLynx XS Application Manager with ACQUITY UPLC I-Class and Xevo® TQ-S micro.

USABILITY

Work intuitively with mass spectrometry

The user interface in MassLynx ensures direct, intuitive access to the functionality that you use most. The result is a user-friendly and fully comprehensive solution that will increase laboratory productivity.

The MassLynx toolbar, displayed alongside the Sample List, provides access at the click of a mouse to instrument status, sample queue information and Application Managers. You can easily switch from viewing the queue to viewing instrument status, or use the tabs to move between general and application-specific tools.

The ability to access basic sample information and system functionality through the MassLynx toolbar allows a novice user to successfully operate the system with a minimal learning curve.

This straightforward interface also gives the experienced user fast access to the advanced features MassLynx offers for sophisticated experiments.

VERSATILITY

Complete system solutions for sophisticated MS analysis

Waters combines the benefits of chromatographic separation and mass spectrometry as a powerful analytical technique, seamlessly controlled by a single software platform.

Together our instruments, software, chemistries, and comprehensive service and support bring you an integrated system that yields high sensitivity, robustness, and versatility.

GET THE MOST FROM YOUR HARDWARE, WITH SEAMLESS SOLUTIONS FOR ADVANCED APPLICATIONS

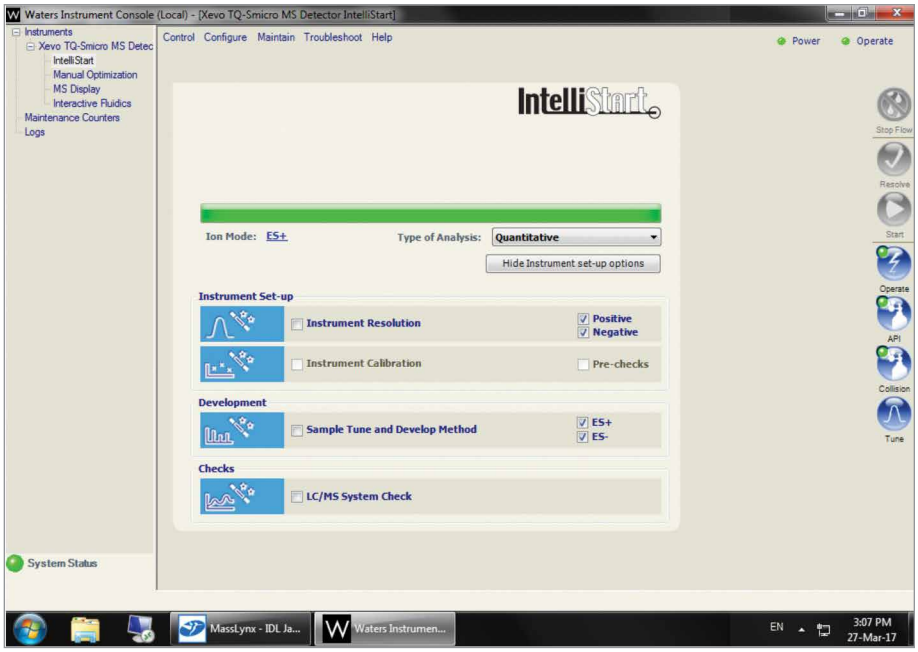
- Collect nominal or accurate mass MS and MS/MS data.
- Streamline data acquisition and processing.
- Acquire both low- and elevated-energy mass spectra with MS^E
- Real-time Data Directed Analysis (DDA™) allows you to automatically switch from MS to MS/MS acquisition when a compound of interest is detected.
- On-the-fly, automated accurate mass measurement using the internal reference standards from the LockSpray™ Source for Tof-MS systems.
- i-FIT™ algorithm for the Elemental Composition Calculator enables you to shorten predicted formulae lists for structural prediction in exact mass measurements.
- Control ionization sources including ESI, APCI, Multi-Mode Ionization, UniSpray,™ APPI/APCI Dual Ionization, DESI, ASAP, APGC, and MALDI.
- Supports Waters and third-party inlets, autosamplers, and detectors.

Improved system interaction

The real power of MassLynx lies in its ability to intelligently control an entire Waters MS system – from the sample and solvent management components to the mass spectrometer and auxiliary detectors. With an embedded PC acquisition system (EPCAS™), MassLynx puts intelligence and real-time functionality inside every mass spectrometer.

MassLynx features IntelliStart™ for Waters MS Systems. IntelliStart integrates internal calibration fluidics and advanced diagnostics software, allowing the system to automatically tune, calibrate, and conduct full UPLC-MS/MS performance checks.

MassLynx provides intuitive data processing workflows for high-performance analytical instruments. This eliminates the complexity that can be associated with high-resolution MS and ion mobility data.



MassLynx IntelliStart user interface integrates fluidics management with diagnostics software, allowing the system to automatically tune, calibrate, and conduct full UPLC-MS/MS performance checks. All you need to do is run your sample.

COMPLIANCE

MAINTAINING SECURITY IN A REGULATED ENVIRONMENT

Strictly regulated laboratory environments place significant demands on LC-MS, LC-MS/MS, and GC-MS systems to maximize performance while also maintaining the security of data.

The MassLynx security system provides compliance-ready tools to meet GxP and 21 CFR Part 11 regulations. It is built on the latest file encryption, audit log, and secure archival/retrieval technology, and has been optimized for convenience and ease-of-use. The flexibility of the security system allows you to tailor and deploy security policies that meet the requirements of your laboratory.

- **MassLynx Security Manager**
  Allows you to configure access privileges for each user, enabling you to easily deploy operator, administrator, and maintenance policies to meet your existing security protocols. Multiple user groups with access to alternative project areas are permitted fully-secured operation when required, and operation in less restrictive projects with less restrictive privileges when appropriate.
- **Secure file encryption**
  Employs the latest encryption and checksum technologies to prevent accidental or deliberate tampering with files. An optional component of the secure file system is the addition of electronic signatures.
- **Audit log**
  Provides an un-editable, hidden, encrypted file that automatically records all log-on and log-off events, security policy changes, MassLynx program module activity, and all events which relate to file generation or manipulation. This log file can be viewed and searched using LogLynx.™ In addition to the audit log provided by the MassLynx security system, the TargetLynx XS Application Manager has a detailed audit log that records the specifics of quantitative data processing.
- **Secure archival and retrieval**
  Provides the ability to archive and then restore secure data without compromising date and file integrity.

MassLynx integrates a complete Waters system, such as benchtop Xevo G2-XS QTof and ACQUITY UPLC I-Class for accurate mass measurement. Through MassLynx, you have complete control of the system itself, as well as the data processing tools you need to efficiently convert data into meaningful information.

ADVANCED DATA MANAGEMENT

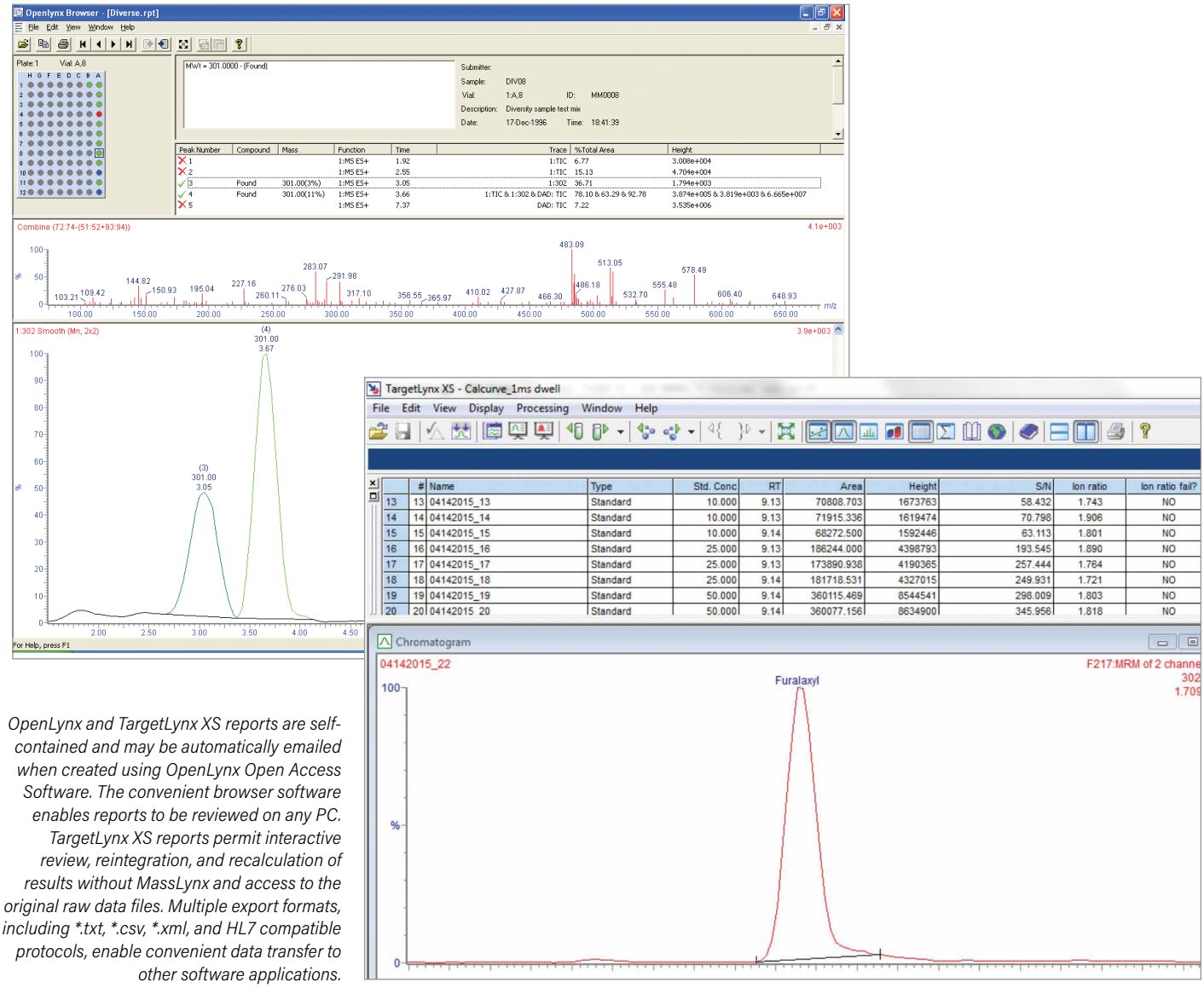
OpenLynx and TargetLynx XS Application Managers

OpenLynx and TargetLynx XS Application Managers are included with MassLynx. The OpenLynx Application Manager allows for customizable batch processing of qualitative MS information. OpenLynx includes quality control capabilities to ensure satisfactory system operation. The OpenLynx browser window facilitates review of large quantities of data; with its convenient plate viewer you can see at a glance whether individual wells contain the target analyte.

The TargetLynx XS Application Manager enables you to perform batch quantification, relying on our ApexTrack™ peak detection algorithm for optimized peak detection and integration. The TargetLynx XS browser contains all information required to review integration, calibration, and quantitation results. You may manually modify integration, enable and disable calibration points as needed, and recalculate the results following review. The internal audit log with configurable reasons for change and electronic signatures supports compliance with applicable regulations.

The comprehensive compliance tools allow for file generation, processing, reporting, archival, retrieval, and audit trails, with the ability to handle electronic signatures.

Data portability



*OpenLynx and TargetLynx XS reports are self-contained and may be automatically emailed when created using OpenLynx Open Access Software. The convenient browser software enables reports to be reviewed on any PC. TargetLynx XS reports permit interactive review, reintegration, and recalculation of results without MassLynx and access to the original raw data files. Multiple export formats, including *.txt, *.csv, *.xml, and HL7 compatible protocols, enable convenient data transfer to other software applications.*

FOR TARGETED ANALYSES

TargetLynx XS

Quantifying and confirming, TargetLynx XS delivers the information necessary for regulatory compliance. With a full range of automatic quality control checks for flagging out-of-range data, TargetLynx lets you identify at a glance samples that fall outside user-specified or regulatory thresholds.

QuanOptimize

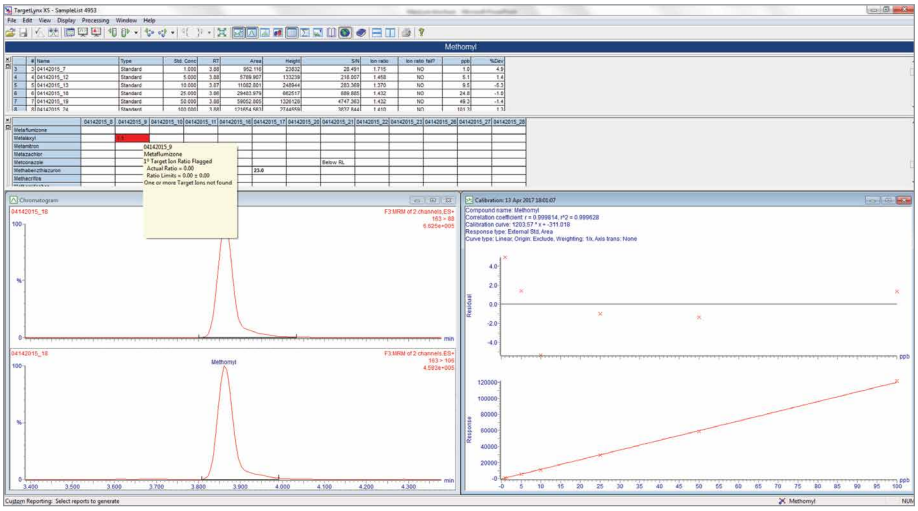
Automating MS and MS/MS method development, QuanOptimize™ delivers high performance, high throughput quantification. Automated instrument optimization doesn't stop at cone voltage, collision energy and MRM transition selection – QuanOptimize also identifies the best ionization method for each compound (ESI or APCI, positive or negative) and automatically quantitates and reports your batch.

OpenLynx Open Access Login

For walk-up analysis, OpenLynx Open Access Login offers multi-user and unsupervised sample login, backed by centralized system management.
For LC-UV, LC-MS, LC-MS/MS, and GC-MS sample runs, from data acquisition to batch processing for qualitative and quantitative analysis, use OpenLynx to fully automate all stages in LC-MS quantification.

FractionLynx

Automating compound isolation and purification, FractionLynx™ controls fraction collection while tracking sample, fractions, and associated data. All possible through integrating versatile control of purification systems with an extensive and flexible set of compound detection, fraction triggering, and collection capabilities.



Example of TargetLynx XS browser showing processed data.

FOCUS THE POWER OF MS ON YOUR APPLICATION

The rate-determining step in many analyses is not data acquisition, but the speed your data can be converted into useful information.

To assist with both application specific data acquisition and the transformation of data into usable results, MassLynx offers Application Managers with specialized data processing functionalities that allow you to eliminate complex, time consuming manual data review.

FOCUS THE POWER OF MS ON YOUR LABORATORY TASKS AND INCREASE YOUR PRODUCTIVITY

The functionality of MassLynx Application Managers was guided by recommendations from our customers. We worked closely with labs like yours to better understand unique MS data processing challenges.

We developed these software extensions to improve your ability to control, collect, and process MS data for specific laboratory needs. The OpenLynx and TargetLynx XS Application Managers are included with each MassLynx installation.

FOR IDENTIFICATION

ChromaLynx XS

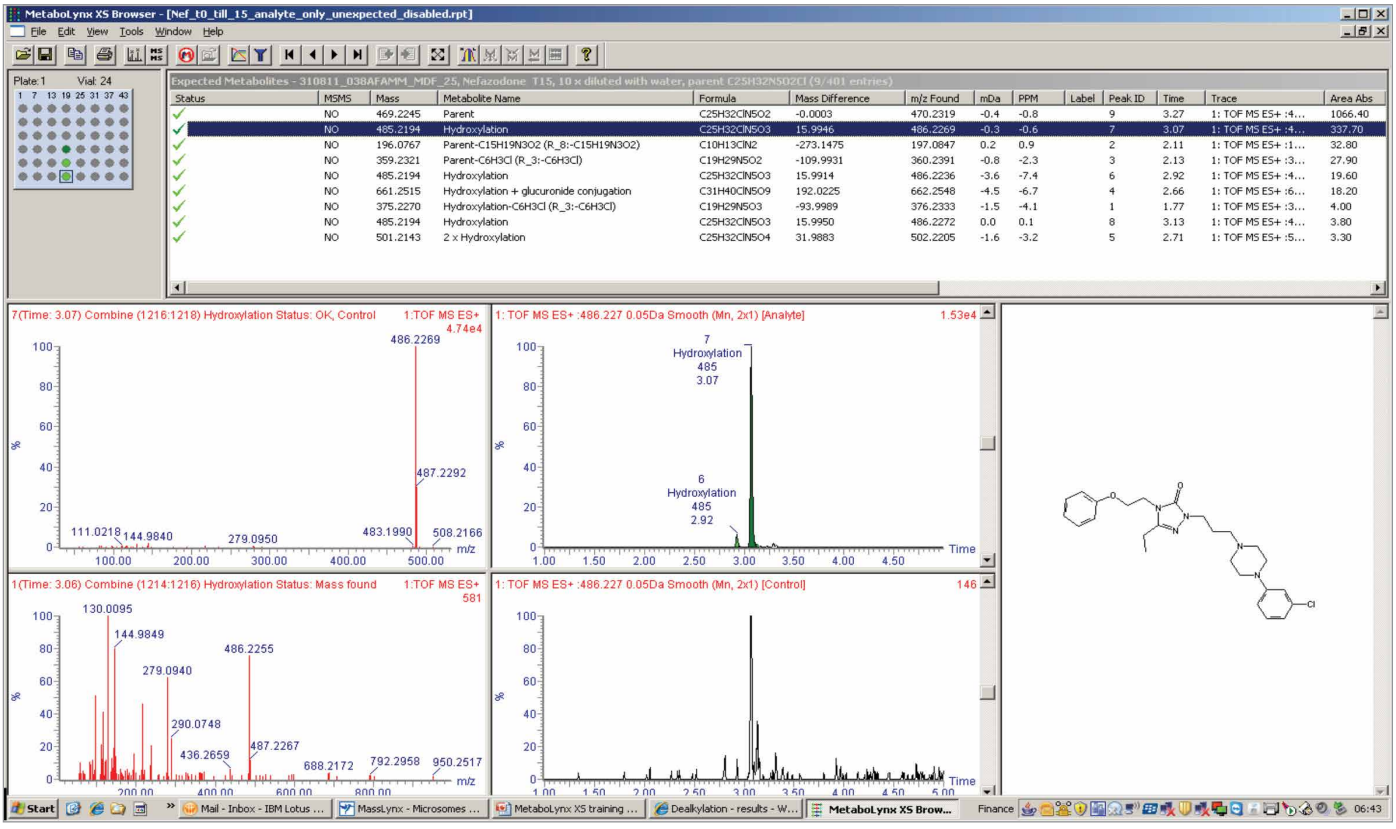
Simplifying complex mixture analysis, ChromaLynx™ XS excels at semi-quantitative detection, identification and determination of components. Detecting and locating the maximum number of real components in a mixture, ChromaLynx also provides comparisons between a real sample and a blank to help determine common and unique components.

MetaboLynx XS

Automating metabolite identification, MetaboLynx™ XS leverages advanced comparison with control samples. You'll miss fewer metabolites and accelerate your data interpretation. Advanced mass defect filters (MDF) let you concentrate on unexpected metabolites while the structural elucidation capabilities of MassFragment™ delivers the information you need to resolve metabolic pathways.

MassFragment

Automatically assigning collisionally activated dissociation mass spectra, MassFragment employs a novel systematic bond dissociation approach, rather than the traditional rule-based and rule-limited approach, delivering confident structural elucidation of your compounds.



MetaboLynx XS automates data processing for rapid metabolite identification. The unique structural elucidation capabilities of MassFragment for MetaboLynx interpret the enhanced fragment information from the SYNAPT® HDMS® for the most advanced characterization capabilities in small molecule profiling.

FOR BIOPHARMACEUTICAL IDENTIFICATION AND CHARACTERIZATION

BiopharmaLynx

Developed for confident characterization and optimized workflow, BiopharmaLynx™ leverages Waters' leading protein informatics expertise. Determine the identity, purity, and stability of biopharmaceuticals, working with either peptide maps or intact proteins.

INTEGRATION WITH INFORMATICS SOLUTIONS

MassLynx is part of the Waters Laboratory Informatics suite, which offers complete solutions to improve your laboratory's ability to capture data, secure information, and share knowledge. MassLynx offers tight, automated integration with our laboratory informatics solutions:

Progenesis QI

Progenesis® QI and Progenesis QI for proteomics enable you to accurately quantify and then identify the compounds and proteins in your omics samples that are significantly changing. Our unique approach to co-detection of compound ions is vital for accurate and precise quantification and access to a wide variety of search methods such as LipidBlast, ChemSpider and Elemental Composition gives great flexibility. Powerful data visualization's and a guided-workflow give ease of use and great confidence in experimental results.

LiveID

LiveID™ Software enables the real-time classification of samples using direct analysis MS data. Compounds are measured in an unbiased fashion providing a holistic view of the sample. Initially, authentic verified samples are used to create and validate a multivariate statistical model. Validated models are then used to test samples to generate live classifications. The output is a simple yes/no answer.

Symphony

Symphony™ Software is a client/server application that is triggered by a MassLynx acquisition and allows the automation of one, or several, post-acquisition data processing functions in a sequence. It is built with efficiency, flexibility, and creativity in mind and enables laboratories to extract maximum value from LC-MS instrumentation.

NuGenesis Lab Management System

NuGenesis® LMS has multiple points of integration with Masslynx. The Scientific Data Management System (SDMS) within NuGenesis LMS provides capabilities to manually or automatically capture reports from MassLynx and archive the data files generated by the MassLynx application. In addition to the data management functionality, NuGenesis LMS Connectors can automate the bi-directional communication of sample and result data to MassLynx with laboratory business systems like SAP and other commercially available LIMS systems.

WATERS GLOBAL SERVICES

Delivering world renowned services and support

Waters Service and Support offerings are tailored to optimize your laboratory productivity while addressing your budget realities. Our offerings help maintain system peak performance, minimize down time, address scientific application challenges, and support stringent compliance requirements. As your services and support provider, we are committed to the success of your laboratory and business.

Waters quality support and consultative services ensure your success wherever your laboratory is located in the world.

Confirmit
ACE AWARDS
Achievement in Customer Excellence

Waters has consecutively earned the ACE Award since 2001 for providing best-in-class technical knowledge, issue resolution, and process support.

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