![Shimadzu - Excellence in Science]

Quadrupole Time-of-Flight Liquid Chromatograph Mass Spectrometer

LCMS-9030

Effortless Performance

The LCMS-9030 quadrupole time-of-flight (Q-TOF) mass spectrometer integrates the world' s fastest and most sensitive quadrupole technology with TOF architecture. A product of Shimadzu's engineering DNA, speed and effortless performance enable the LCMS-9030 to address qualitative and quantitative challenges with genuine confidence and ease.
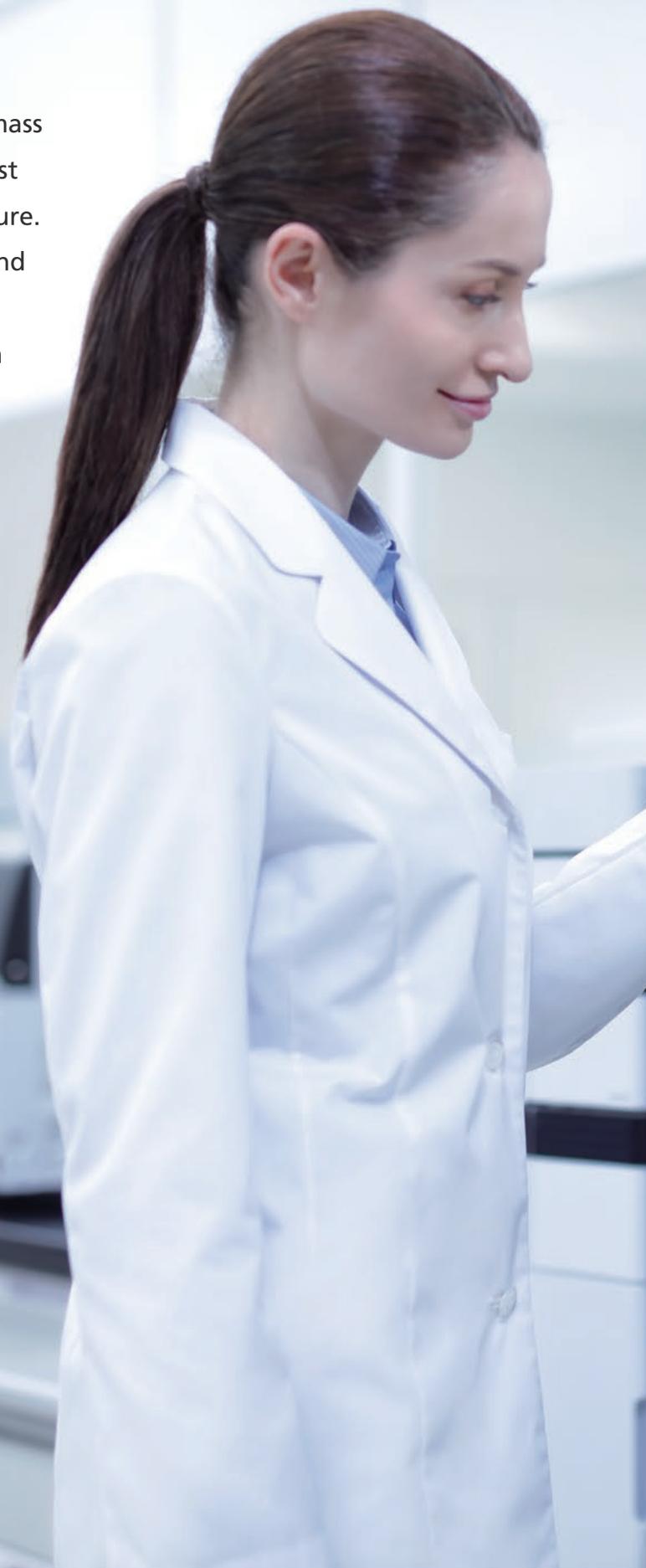
Watch the product video on our website.

Quadrupole Time-of-Flight
Liquid Chromatograph Mass Spectrometer

LCMS-9030

Greater Accuracy

Better Sensitivity

Higher Resolution

iF DESIGN AWARD 2019

SHIMADZU

LCMS-9030
LIQUID CHROMATOGRAPH MASS SPECTROMETER

Key Technologies of the LCMS-9030

The LCMS-9030 uses newly patented technologies to deliver both high resolution and accurate mass, attributes essential for confident formula assignment and unknown identification. The high-efficiency ion guides, quadrupole, and collision cell enable high sensitivity for the detection of trace-level compounds. Unique UFgrating and iRefTOF technologies ensure ultrafast acceleration of ions into the flight tube (UF-FlightTube) and ideal reflection of those ions back to the detector. The result is high-speed data acquisition compatible with the high-throughput laboratory.

▶▶ High-Efficiency Quadrupole Technologies

UFsweeper™ III Collision Cell

Quadrupole

UF-Lens™

UF-Qarray™

DL (Desolvation Line)

Heated ESI Probe

MCP

Sub-Interface
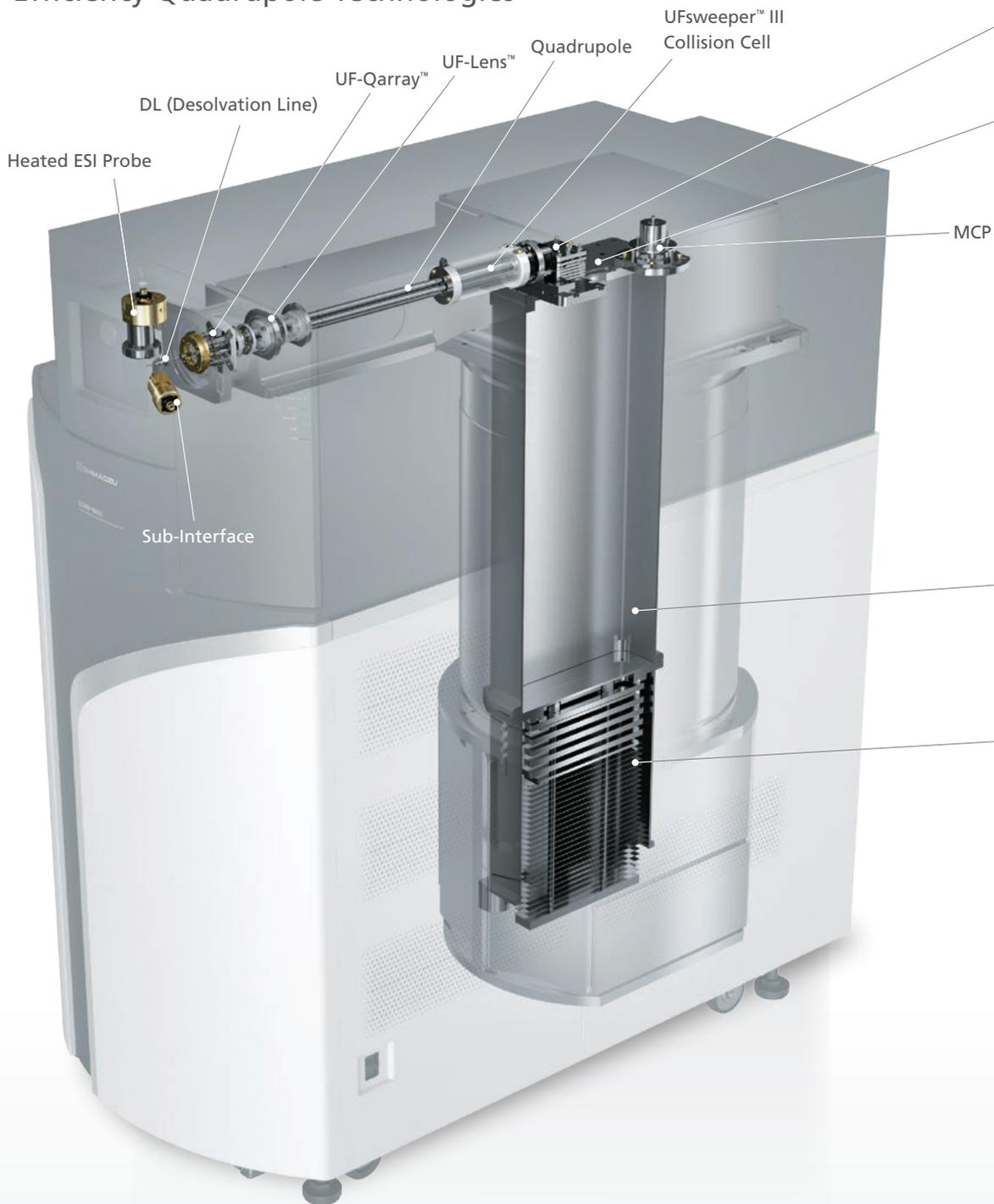
▶▶ New TOF Technologies

UFaccumulation™ (Pat. US 10020181)

Ion accumulation in the collision cell, synchronized perfectly with short cycles of data acquisition, maximizes sensitivity.

UFgrating™ (Pat. US 9048082)

Shimadzu's world-class manufacturing capability has enabled the ion acceleration electrode to be made with substantial mechanical strength. This grating is able to withstand the high voltages needed for ultrafast ion pulsing.

Traditional mesh electrodes for ion transmission lack mechanical strength, limiting acceleration voltage.

Shimadzu's UFgrating has superior mechanical strength over conventional electrodes.
  This unique grating structure makes it possible to apply a higher voltage.
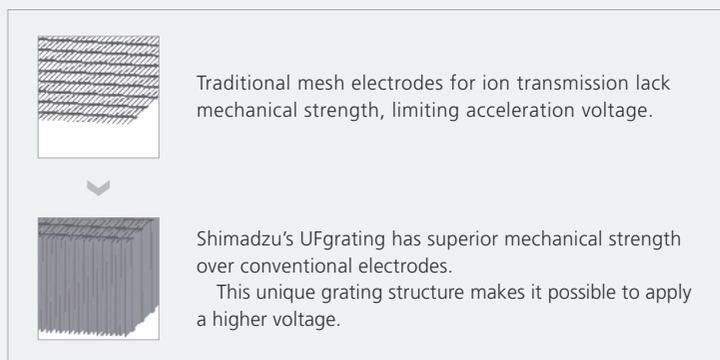
UF-FlightTube™ (Patent Pending)

With excellent architecture, the UF-FlightTube prevents and withstands subtle deformations caused by temperature changes, affording stability of performance.

iRefTOF™ (Pat. US 8772708, 9490114)

A computationally ideal electrostatic field has become a reality. Meticulously manufactured plate electrodes are stacked to create a reflectron that compensates for the energy distribution of ions with no compromise in either resolution or sensitivity.

UFgrating   MCP

iRefTOF

A Slim, Floor-Standing Design

The simple and compact design conserves valuable laboratory space.

Effortless Performance for Accurate Mass

Excellence in Mass Measurement Accuracy (MMA)

Mass measurement accuracy (MMA) is the key performance attribute underlying all application fields using high-resolution accurate-mass (HRAM) spectrometers. The LCMS-9030 delivers the MMA needed for high-confidence identification of unknown compounds at an unprecedented level of stability. This is made possible by new technologies implemented in the Intelligent Temperature Control System and the UF-FlightTube that accurately offset the changes occurring to both internal and external environments. With the LCMS-9030, Shimadzu aims to totally refashion the HRAM user experience, enabling scientists to run more samples at longer calibration intervals with greater confidence and ease.

Intelligent Temperature Control System (Patent Pending)

Stable MMA Against Temperature Fluctuation

Shimadzu's Intelligent Temperature Control System ensures stable MMA even in laboratory environments susceptible to temperature changes. To demonstrate, standards ranging from 150 to 1700 Da were analyzed continuously after a single calibration. Normal laboratory temperature fluctuation was observed between 25°C and 28°C.

Without additional mass correction, the measured accurate masses of all compounds remained within 1 ppm of the theoretical mass for the 60-hour duration of the experiment. With the LCMS-9030, laboratory productivity can be increased by running long, calibration-free batches with confidence.

Positive Mode
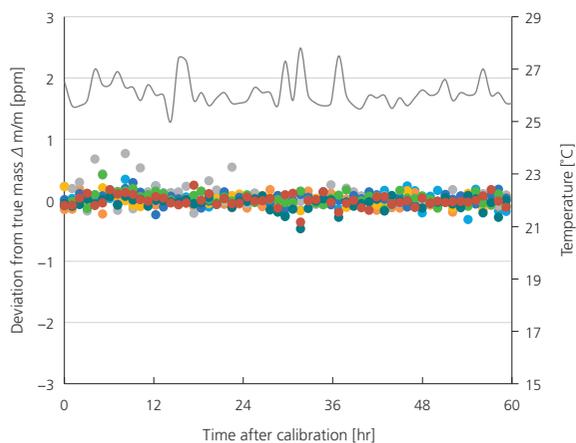
Legend:
- Acetoaminophen
- Progesterone
- Griseofulvin
- Rifampicin
- Temperature
- Anisomycin
- Mitomycin C
- Doxorubicin
- Valinomycin

Negative Mode

Legend:
- Doxorubicin
- Thiostrepton
- Valinomycin
- Temperature
- Salinomycin
- Tubercidin
- Mitomycin C
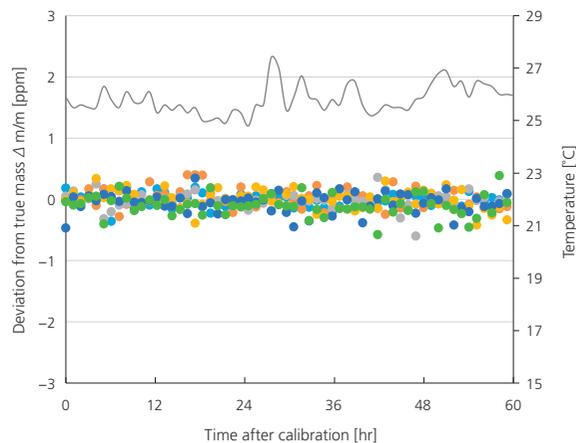
High MMA Over Wide Concentrations

The LCMS-9030 breaks new ground for quantitative analysis not only by its high sensitivity but also by the selectivity afforded by high MMA over a wide range of concentrations. Genuine ion statistics ensure that all measurements throughout the peak elution result within a narrow *m/z* window of the extracted ion chromatogram (XIC), as shown below for Verapamil analysis. Even at 10 fg injection, the overall mass

error was less than 1 ppm and all data points gave results within the 5 ppm XIC window for accurate, repeatable and selective quantitation. Moreover, stability of MMA allows the same XIC setting to be comfortably used for series of analyses.

XIC of Verapamil [M + H]⁺ (exact mass 455.29042)
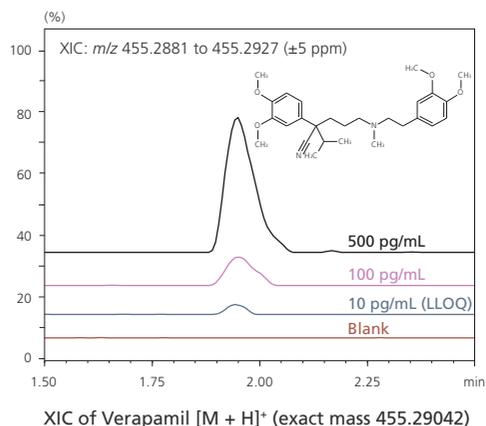
Quantitative Results of Verapamil

Conc. (pg/mL)	Calculated conc. (pg/mL)	Area RSD (%, n = 3)	Accuracy (%, n = 3)
500	523.3	1.93	104.67
100	96.3	3.78	96.50
10 (LLOQ)	10.3	5.31	100.50
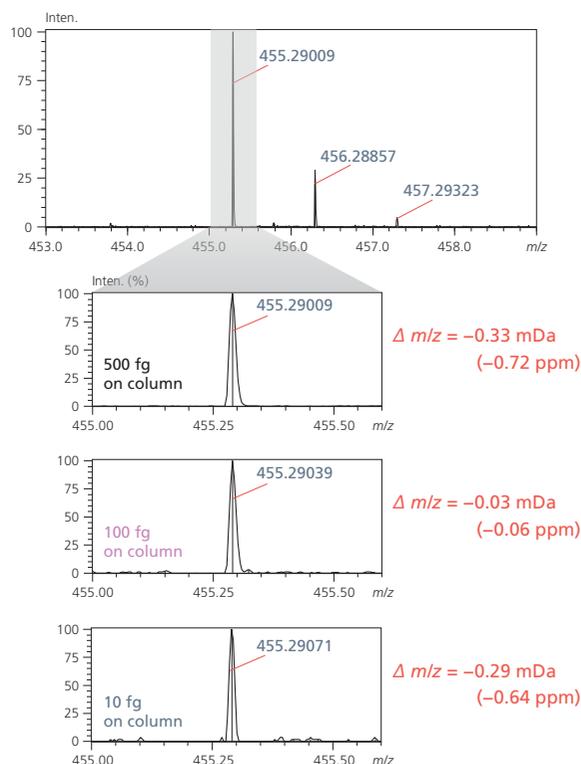
Averaged Mass Spectrum at Each Concentration

Same MMA Across Acquisition Modes

MS/MS spectra are a key tool for structural elucidation of unknown compounds, and ease of data interpretation is directly dictated by the MMA of MS/MS acquisition. This makes the LCMS-9030 an ideal instrument for structural analysis as its MS/MS mode achieves equally high MMA as the MS mode, thanks to the collision cell technologies that generate high-abundance fragment ions.
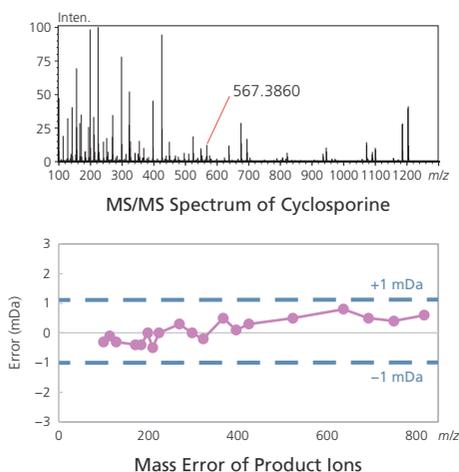
The results of MS/MS structural analysis of cyclosporine are shown below. Numerous ions were matched with putative fragment structures at less than 1 mDa mass error. Formula prediction results for *m/z* 567.3860 at different mass error tolerances demonstrate the impact of MS/MS MMA in making the prediction unambiguous.

MS/MS Spectrum of Cyclosporine

Mass Error of Product Ions

Predicted formula: C28H51N6O6
Theoretical *m/z*: 567.3865
Mass error: 0.88 ppm (0.5 mDa)

Formula Prediction Results for *m/z* 567.3860

LCMS-9030
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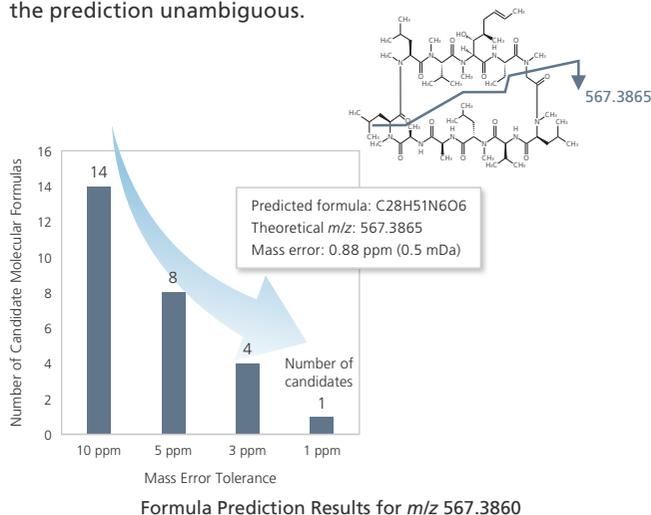
HRAM for Selective Detection of Isobaric Compounds

The LCMS-9030 produces the high-resolution accurate mass data needed to distinguish between compounds having the same nominal mass. Three isobaric compounds, 4-Hydroxytriazolam, α-Hydroxytriazolam, and α-Hydroxy-etizolam, were analyzed in whole blood at 10 ng/mL.
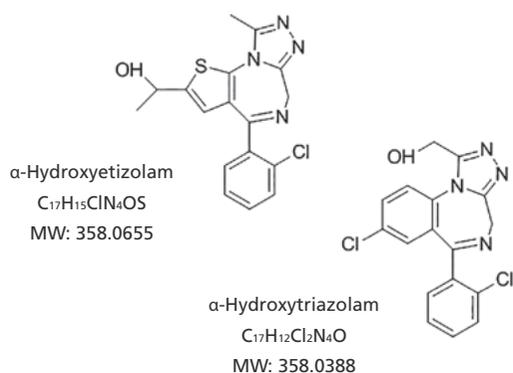
Even with incomplete chromatographic separation, each compound was detected as an isolated ion without cross talk. Another isobaric pair, Triazolam and Etizolam, also demonstrates the ability of the LCMS-9030 to isolate ions that differ by only 0.0267 amu. Quantitation can be improved by the isolation of analytes from isobaric interferences.

α-Hydroxyetizolam
$C_{17}H_{15}ClN_4OS$
MW: 358.0655

α-Hydroxytriazolam
$C_{17}H_{12}Cl_2N_4O$
MW: 358.0388
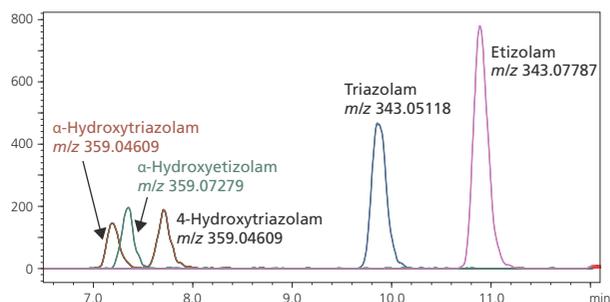
LCMS-9030 Mass Chromatogram of Etizolam, Triazolam, and Metabolites Spiked at 10 ng/mL in Whole Blood.

Design Compatible with Shimadzu's Triple Quadrupole Line

Method transfer between the LCMS-9030 and Shimadzu's triple quadrupole product line is easy and effective because Shimadzu's LCMS products share related technologies for the heated ionization source, ion focusing optics, and collision cell. This means that key method parameters like ESI source conditions, lens voltages, and collision energy are compatible between systems. The LCMS-9030 is built on the high-sensitivity ion technologies of the triple quad LCMS-8060, and produces similar high-quality spectra.

To make Data Dependent Acquisition (DDA) settings easy, the LCMS-9030 uses an automated range of collision energies for effective fragmentation. Shimadzu's CE Spread function allows the user to obtain high-quality MS/MS spectra even when the optimal collision energy is not known. In the example below, the Q-TOF spectrum obtained with the CE Spread function is compared with the merged spectrum from a series of discrete collision energies obtained on the LCMS-8060. The excellent agreement of the results demonstrates the high-quality spectra that can be obtained from Q-TOF DDA experiments.

Product Ion Spectra of Etizolam

Etizolam
$C_{17}H_{15}ClN_4S$
$[M + H]^+ = 343.0779$

Cleavage Pattern of Etizolam
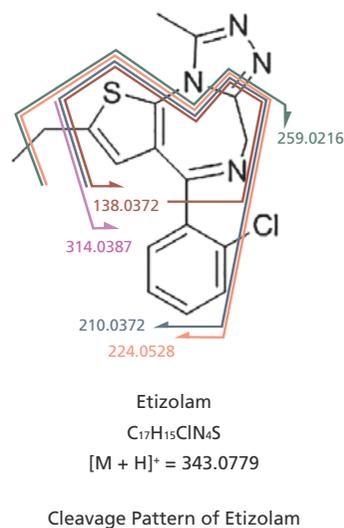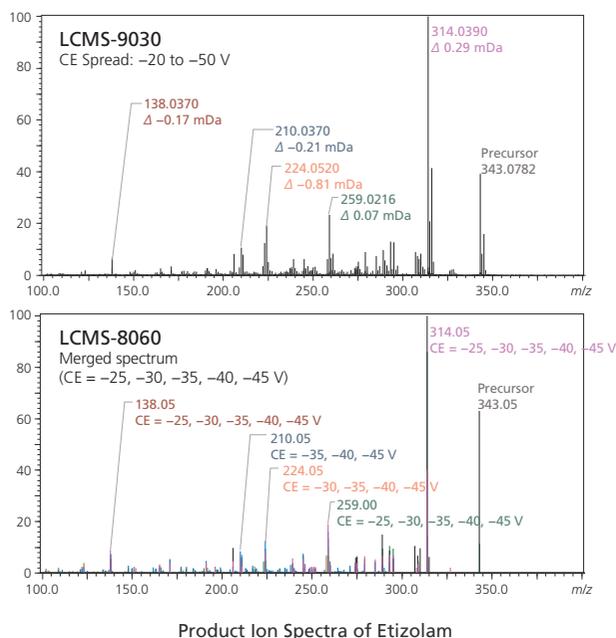
Data Courtesy of Associate Professor Kei Zaitsu
(Nagoya University Graduate School of Medicine)

Ionization Units

In addition to the standard ESI ionization unit, optional APCI and Dual Ion Source (DUIS) probes are available for the LCMS-9030 to meet various analytical needs. Shimadzu's DUIS offers an efficient combination of ESI and APCI ionization capabilities.

ESI (standard)

APCI (optional)

DUIS™ (optional)

The dual ion source continuously performs both electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI).

Calibrant Delivery System (CDS)

The CDS allows calibration standards to be introduced via a separate ionization probe that functions independently from the main probe. This optional sub-ionization unit is installed in the main probe housing and is available for all probe types (ESI/APCI/DUIS). By having two probes in one system, high-concentration calibration standards can be introduced only when needed without switching flow lines, and are kept in isolation from the sample stream, eliminating contamination.
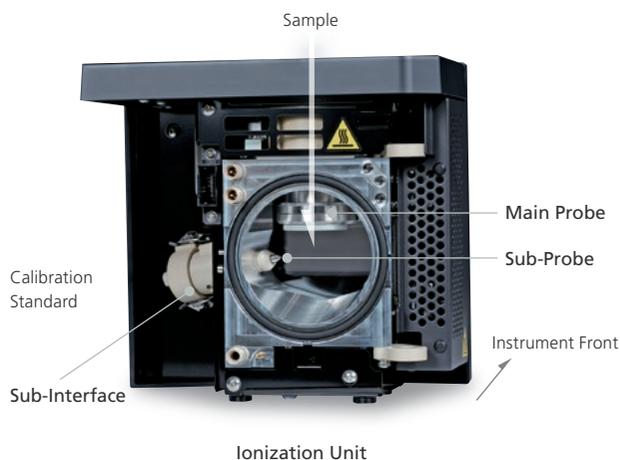
Ionization Unit

Micro-ESI 9030 Micro-flow Ionization Unit

Shimadzu's Nexera Mikros microflow system combines the sensitivity improvements you expect from a low-flow system with the ruggedness of HPLC. Designed for optimal sensitivity and ease of use, the Micro-ESI 9030 interface brings microflow analysis to the Q-TOF. Ionization efficiency and transfer have been maximized by the probe design, resulting in high sensitivity, stable operation, and minimal contamination. To minimize dead volume and diffusion, the Nexera Mikros features an innovative snap-in column locking system, the UF-Link™, allowing any user to correctly install a microflow column without disrupting the ESI spray needle position. Realize the benefits of microflow while enjoying the reliability of HPLC.
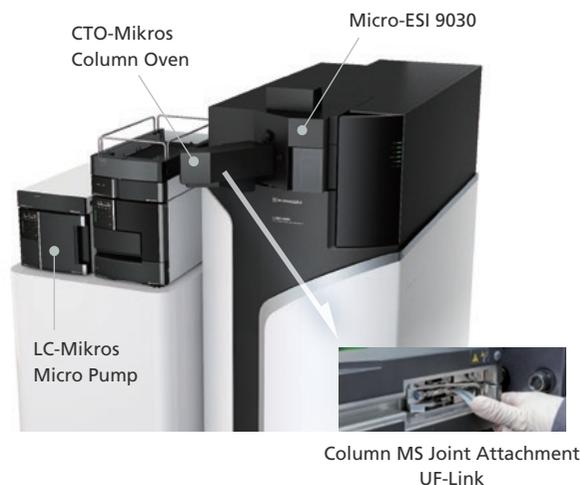

Nexera Mikros & Micro-ESI 9030 System

LabSolutions Insight™ Explore

Software for Both Qualitative and Quantitative Analysis

LabSolutions Insight Explore offers an intuitive and full-featured quantitative environment with significant qualitative enhancements. A sophisticated peak detection algorithm detects chromatographic features based on their accurate mass. Resulting peak displays enable ranked formula prediction with theoretical spectral matching. A deconvolution algorithm is also provided for analysis of polyvalent ions.

Sample List

MS Chromatogram Display Window

MS Chromatogram List

MS Spectrum List

MS Spectrum Display Window

List of Candidate Formulas
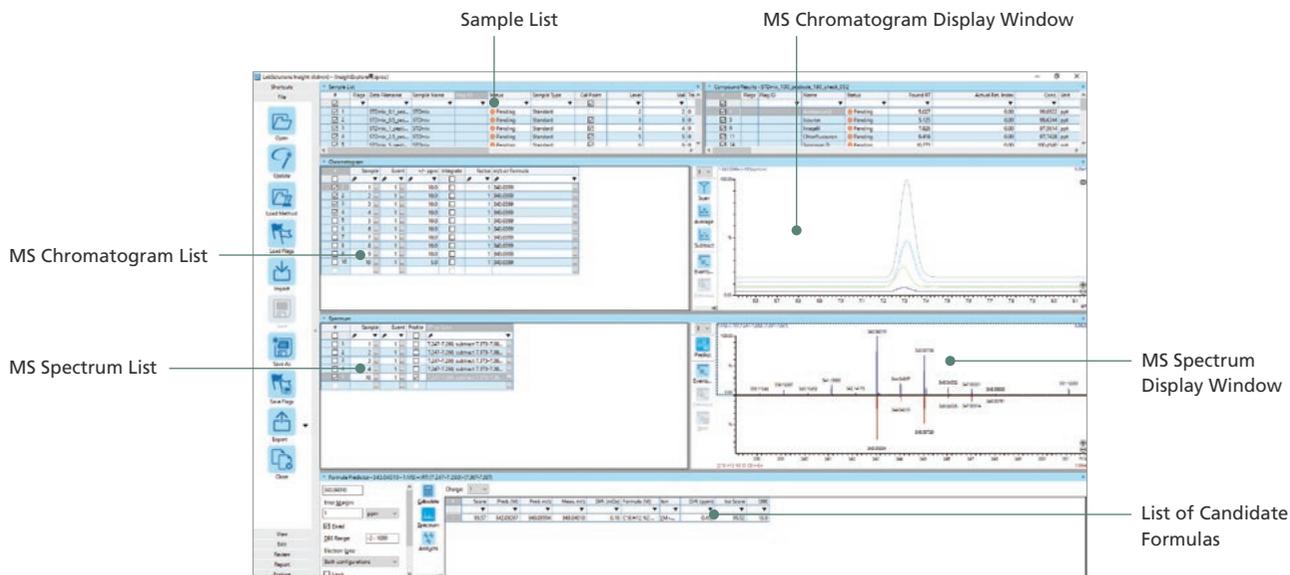
Quantitative Analysis

High-sensitivity MRM (Multiple Reaction Monitoring) analysis performed on the LCMS-9030 can eliminate background interferences by using accurate mass detection. Used together with Shimadzu's ion accumulation feature, extraordinary Q-TOF sensitivity is delivered. Insight provides a complete and flexible quantitative interface with user-defined flags to facilitate review by exception.

Data Results Filtered According to User-Defined Flags

Calibration Curve Information

Chromatogram Display Window
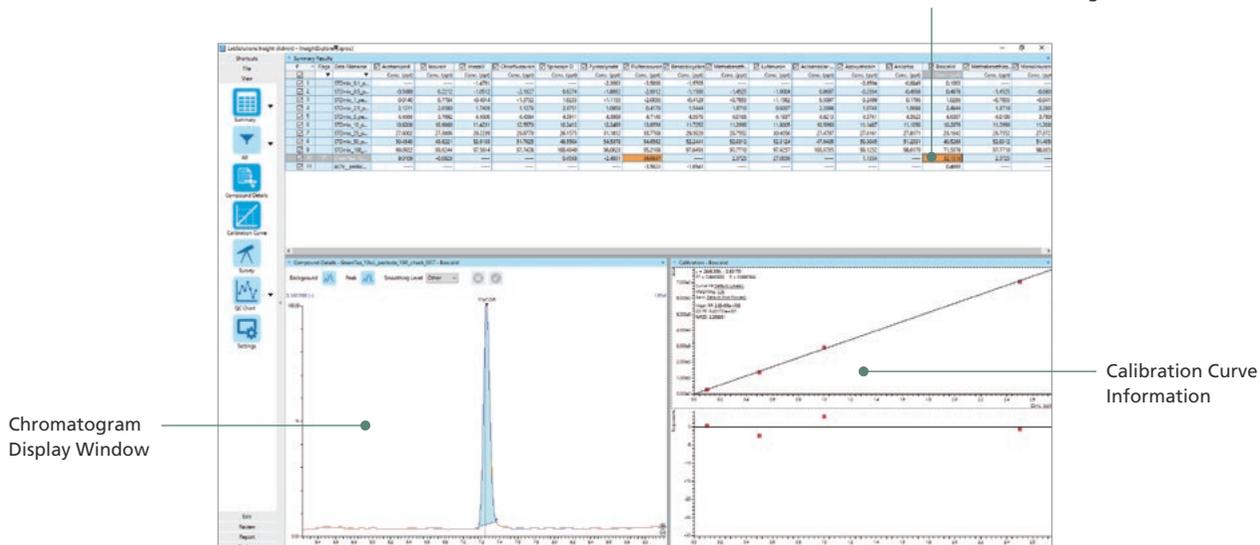
Formula Prediction

To facilitate unknown identification, Insight integrates formula prediction capabilities. High-resolution accurate mass data is utilized to create a list of possible formulas, displayed according to user preference. Theoretical spectra and isotope patterns can be used for putative identification. In the example below, the pesticide Boscalid was identified in a green tea extract.
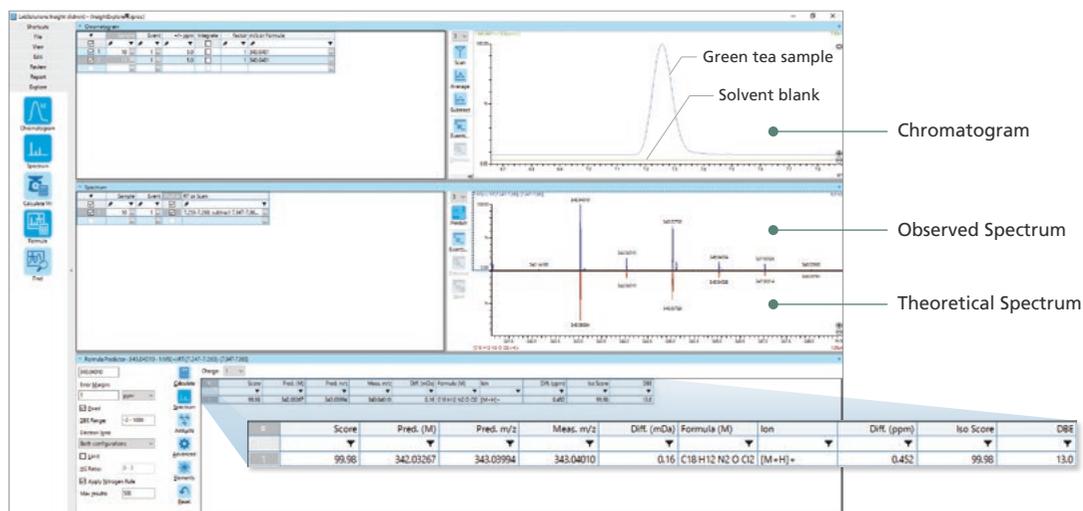

Example of Unknown Identification of Boscalid ($C_{18}H_{12}N_2OCl_2$) in Green Tea

Multivalent Ion Analysis (Deconvolution)

For the deconvolution of multiple charge state envelopes produced by large molecules, such as proteins and oligonucleotides, LabSolutions Insight Explore includes ReSpect. This multivalent ion analysis algorithm from Positive Probability Ltd detects related multi-charged peaks and calculates the mass of the original species. Excellent mass accuracy was obtained in the example below.

Deconvolution Example (Oligo dT20)
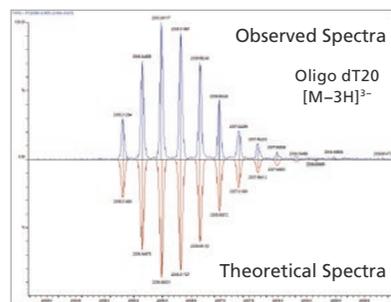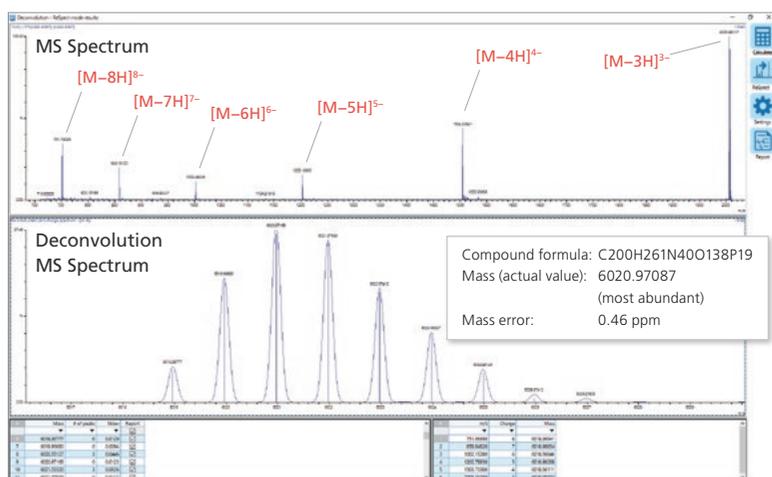
Comparison of Observed and Theoretical Spectra

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