![SHIMADZU logo] **SHIMADZU**

Excellence in Science

Quadrupole Time-of-Flight Liquid Chromatograph Mass Spectrometer

# LCMS-9050

*UFMS*

ULTRA FAST MASS SPECTROMETRY

# Accelerate Discovery

The LCMS-9050 is a Q-TOF mass spectrometer designed for the most reliable and easy acquisition of accurate masses in the real laboratory settings. With the proprietary innovation for fast polarity switching, it has the unique capability for high-confidence identification of challenging compounds and high-throughput screening of multiple unknowns. All sorts of applications are possible by the abundance of optional accessories and front-end configurations that leverage the instrument power.

With the LCMS-9050, Shimadzu introduces a new era in time-of-flight mass spectrometry and continues Shimadzu's tradition of taking on new challenges in LCMS.

# LCMS-9050

Quadrupole Time-of-Flight Liquid Chromatograph Mass Spectrometer

Trusted **mass accuracy**

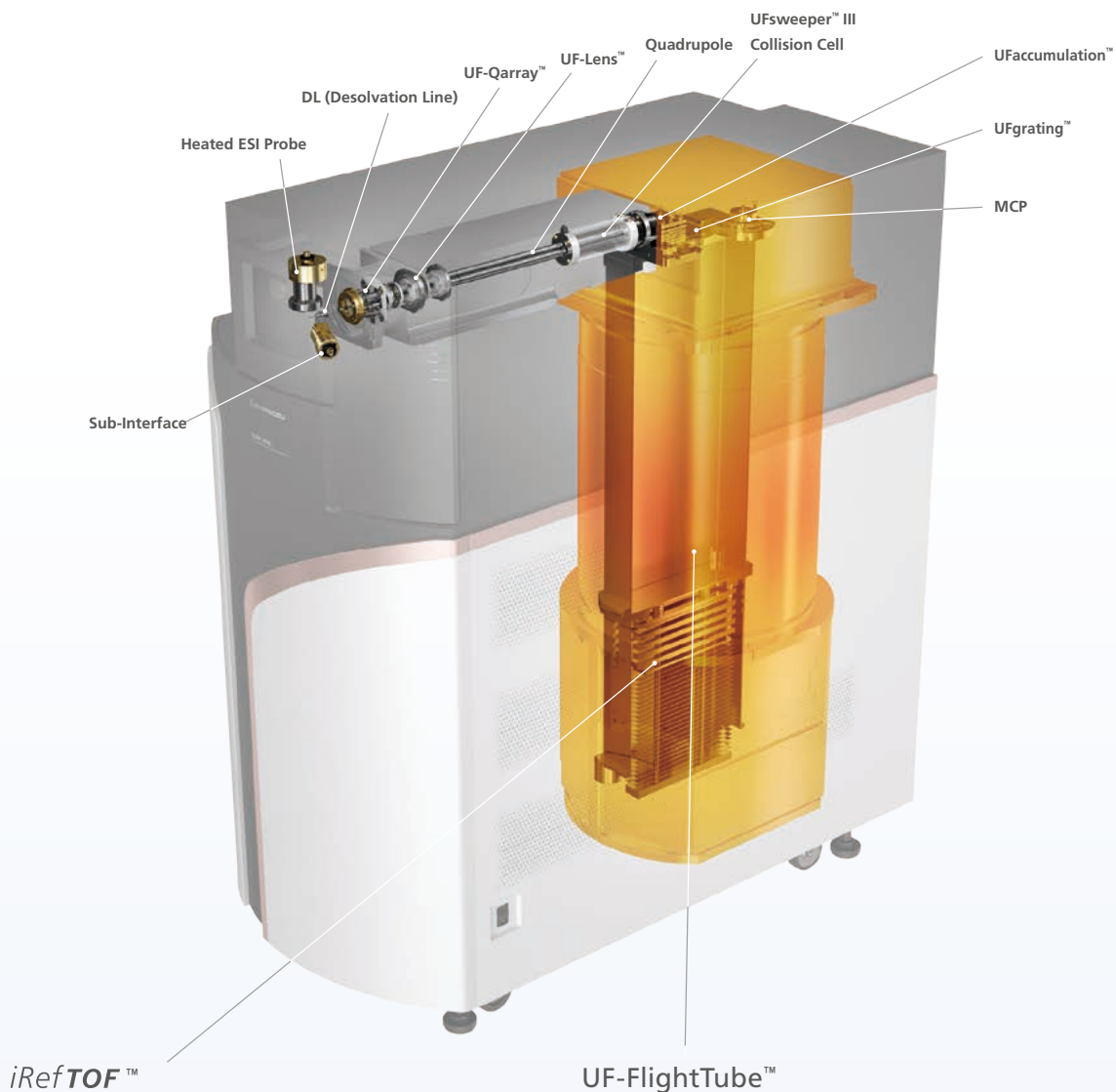Ultra-stable **polarity switching**

Truly versatile with **flexible extensions**

# Trusted mass accuracy

The LCMS-9050 achieves excellent mass accuracy using Shimadzu's unique patented technologies inherited from the LCMS series. Precision temperature control system compensates external factors to sustain good mass measurement accuracies without the need for frequent mass calibration.

## Technologies Inherited from the LCMS Series

Heated ESI Probe

DL (Desolvation Line)

UF-Qarray™

UF-Lens™

Quadrupole

UFsweeper™ III
Collision Cell

UFaccumulation™

UFgrating™

MCP

Sub-Interface

### *iRef**TOF**™*

The unique electrode shape achieves an ideal electric potential distribution that increases energy-focusing, while also inhibiting trajectory divergence and flight time lengthening during ion reflection.

### UF-FlightTube™

Precision temperature control is achieved due to an optimized heater and heater sensor layout and a robust control system. That minimizes the effects of any room temperature variations to enable stable mass accuracy over long periods.
It also reduces the time and trouble required for mass calibration.

## Performance Assistant

The LCMS-9050 includes an auto-tuning function that uses a standard sample to automatically correct mass accuracy, resolution, sensitivity, and other parameters. The function includes various tuning modes that can be selected depending on the instrument status, such as the full-tuning mode for tuning the entire system or other modes for tuning only the TOF unit for mass calibration. Auto-tuning can be executed from the LabSolutions™ LCMS platform without configuring any complicated settings. No expertise is needed to ensure that data are acquired with an optimally configured system.

## A Slim, Floor-Standing Design

The simple and compact design conserves valuable laboratory space.

# Ultra-stable polarity switching

Shimadzu's breakthrough innovation challenges the common belief that TOF instruments cannot undergo efficient polarity switching. With the capability to achieve low-ppm mass measurement accuracies in short switching intervals, possibilities are now open to enhance the workflow with greater confidence and ease.

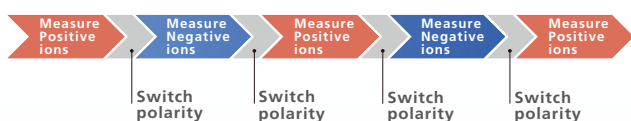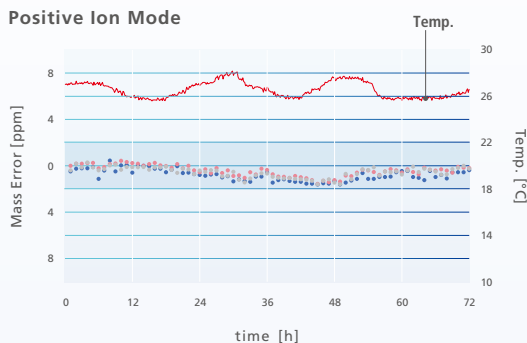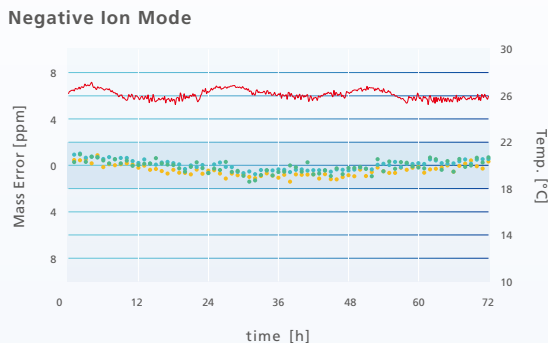## Achieving Both Polarity Switching and Mass Accuracy



Illustration of Switching between Positive and Negative Ion Modes

The LCMS-9050 features a proprietary high-precision electrical circuit and the UFstabilization™ algorithm (patent pending) that make polarity switching both fast and stable.

### Positive Ion Mode



### Negative Ion Mode



### Positive-Negative Switching Mode



● Anisomycin(+)  ● Griseofulvin(+)  ● Valinomycin(+)  ● Doxorubicin(-)  ● Salinomycin(-)  ● Cyclosporine(-)

**Positive ion Mode, Negative ion Mode:** No calibration Mass error was within ±2 ppm even throughout 3 days of continuous analysis.

**Positive-Negative Switching Mode:** External calibration Calibrants were transiently introduced via a sub-interface in between sample analysis for mass correction. The mass accuracy was within ±3 ppm throughout 40 hours of continuous analysis. Both were analyzed under normal laboratory conditions.

**Results of analyzed 6 antibioticcomponents continuously**

The charts on the left each plot the mass errors with respect to theoretical values for six antibiotic components (with molecular weights ranging from 265 to 1203 Da) analyzed continuously under normal laboratory conditions. When three components of antibiotics were analyzed each in positive and negative ion mode, the exact masses of all components showed stable mass accuracy within ±2 ppm of the theoretical values for 72 hours without a single mass calibration. The LCMS-9050's precisely controlled temperature control system minimizes the effects of changes in room temperature and achieves stable mass accuracy without the need for calibration. Mass accuracy (external calibration) within ±3 ppm was obtained for all components in the simultaneous analysis of positive and negative ions. Stable mass accuracy is maintained even during long-time continuous analysis using the positive-negative switching mode.
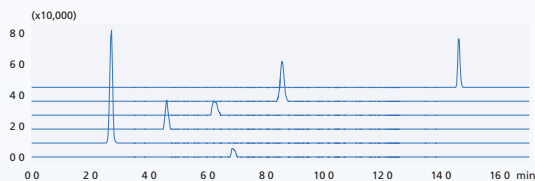
## Increasing Workflow Efficiency with Polarity Switching

Analysis that was previously performed twice in positive ion mode and negative ion mode can now be performed in one analysis, improving the analysis throughput. In addition, positive and negative ions can be detected in the pretreated sample under the same conditions without any time lag, improving the reliability of the analytical data.
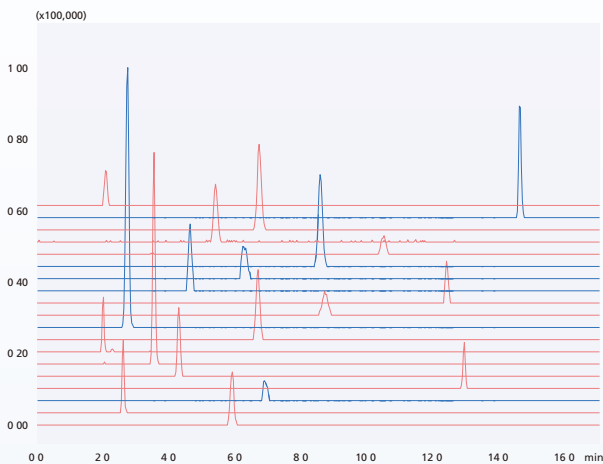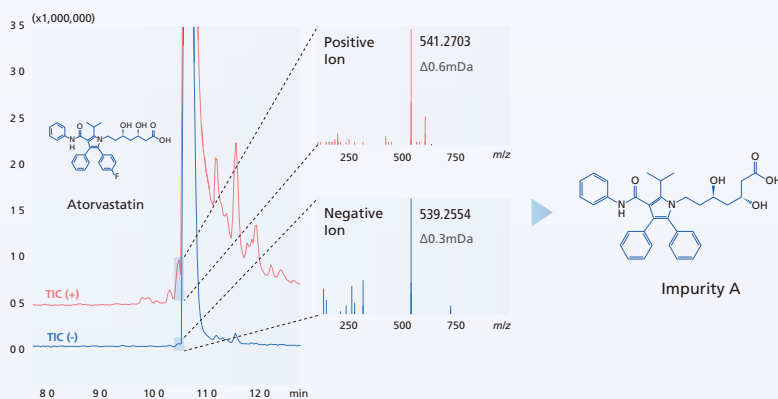
**Positive Ion Mode Measurement**

**Positive-Negative Switching Mode Measurement**
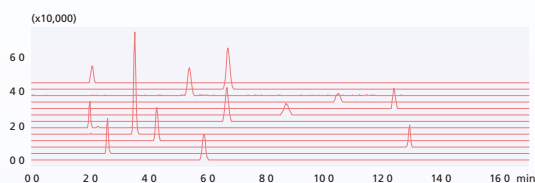
**Negative Ion Mode Measurement**

### Conventional Q-TOF

### LCMS-9050

The positive-negative switching mode was used to analyze a commercially marketed atorvastatin calcium sample. By switching between positive and negative ion modes, both the principal component atorvastatin and the impurities specified in the European Pharmacopoeia (EP) were detected. All were detected with high mass accuracy within ±1 ppm. Measuring in both positive and negative modes provides more information for high-confidence impurity identification.

Positive Ion    541.2703    Δ0.6mDa

Negative Ion    539.2554    Δ0.3mDa

Atorvastatin

TIC (+)

TIC (-)

Impurity A

**Impurity Analysis of Atorvastatin**

# Truly versatile with flexible extensions

A wide variety of analytical challenges can be further addressed by combining the Q-TOF capability with optional ionization units or with unique front-end configurations. These flexible extensions can be easily implemented and switched with little or no intervention of engineers.

## DPiMS™

**Direct Probe Ionization Mass Spectrometer**

A small amount of sample is taken using a probe and directly ionized to measure liquids and solids as they are. There is no need to study LC separation conditions or complicated sample preprocessing. Data acquisition can be completed within 1 minute even if both positive and negative ions are detected. By combining with Shimadzu's Q-TOF, it becomes possible to quickly and easily identify the components in the sample.

Total Ion Chromatograms

Mass Spectrum

## iMScope™

**Imaging Mass Microscope**

This unit is equipped with the laser ionization source and optical microscopy to allow direct comparison of molecular distribution and histological features. In combination with a Q-TOF spectrometer, it enables accurate and fast high-resolution MS image acquisition and analysis.

## CLAM™

**Fully Automated Sample Preparation Module for LCMS**

Simply set up the blood collection tube, and fully automated analysis of blood and urine samples, from pretreatment to LC/MS/MS analysis, is realized, improving workflow efficiency. In order to obtain a full scan of a valuable sample and to collect exhaustive data, Q-TOF is the best combination for this purpose.

## Nexera™ UC

**Supercritical Fluid Extraction / Chromatograph System**

This system uses a supercritical fluid to automatically extract and separate target components. SFC can separate and analyze compounds in a wide range of chemical space, from low to high polarity. Combined with the LCMS-9050's positive-negative switching mode, compounds with a wide range of physico-chemical properties can be analyzed at once, increasing the comprehensiveness of a single analysis.

Using the SFC+LCMS-9050 system, 80 pesticide compounds were simultaneously analyzed using the positive-negative switching mode. The use of supercritical fluid as the mobile phase enables analysis with higher speed, separation, and sensitivity than HPLC. By combining the supercritical fluid system with the high-resolution Q-TOF, the system is powerful for full screening of multiple components.





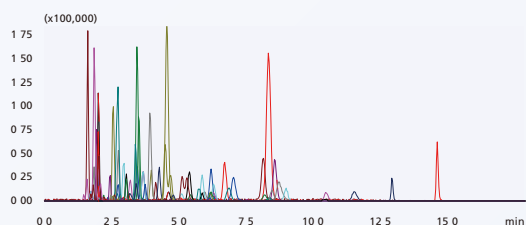**80 components of pesticides Mass Chromatogram**

## Nexera Mikros™

**Supporting Micro Flowrate Range Liquid Chromatography Mass Spectrometry System**

This LCMS system is optimized for low flowrates. Higher ionization efficiency and higher ion-uptake efficiency enable higher sensitivity. In combination with a Q-TOF system, it can be used for comprehensive analysis of trace components.

# LabSolutions Insight Explore™

Explore software not only facilitates quantitative analysis of a large number of samples, but also comes with features for reliable library searching, elucidation of compound structure and sample composition, and multivalent ion analysis, making full use of MS data with high resolution and mass precision.



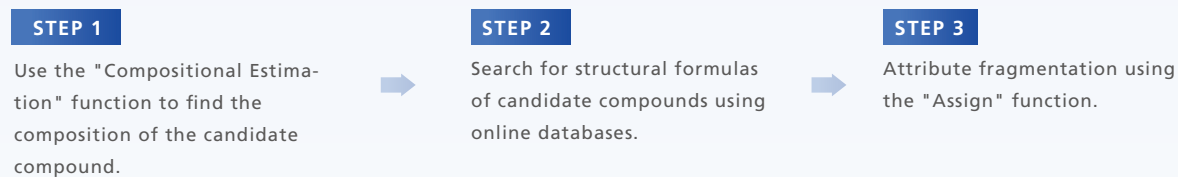## Multivalent Ion Analysis

### (Deconvolution)

For the deconvolution of multiple charge state envelopes produced by large molecules, such as proteins and oligonucleotides, LabSolutions Insight Explore CSD (option) includes "*ReSpect*™". This multivalent ion analysis algorithm from Positive Probability Ltd detects group(s) of multi-charged peaks and calculates the mass of the original species.
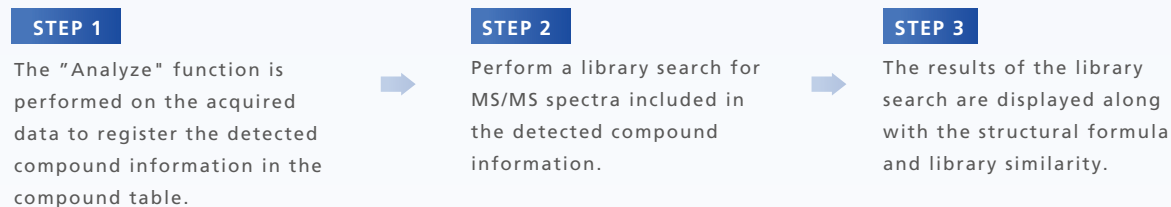
# Data analysis with easy operation

LabSolutions Insight Explore is easy and intuitive to use. Analysis results are visually organized for easy understanding, and all necessary information is presented on a single screen. For example, structural analysis and compound identification by library search can be performed in three steps.

## Structural Analysis Procedure

**STEP 1**

Use the "Compositional Estimation" function to find the composition of the candidate compound.

➡

**STEP 2**

Search for structural formulas of candidate compounds using online databases.

➡

**STEP 3**

Attribute fragmentation using the "Assign" function.

## Compound identification procedure by library search

**STEP 1**

The "Analyze" function is performed on the acquired data to register the detected compound information in the compound table.

➡

**STEP 2**

Perform a library search for MS/MS spectra included in the detected compound information.

➡

**STEP 3**

The results of the library search are displayed along with the structural formula and library similarity.

UFMS, UF-Qarray, UF-Lens, UFsweeper, UFaccumulation, UFgrating, iRefTOF, UF-FlightTube, LabSolutions, UFstabilzation, DPiMS, iMScope, CLAM, Nexera, Nexera Mikros and LabSolutions Insight Explore are trademarks of Shimadzu Corporation or its affiliated companies in Japan and/or other countries.
ReSpect is a trademark of Positive Probability Ltd.

**SHIMADZU**

**Shimadzu Corporation**

**www.shimadzu.com/an/**

**For Research Use Only. Not for use in diagnostic procedures.**
This publication may contain references to products that are not available in your country. Please contact us to check the availability of these products in your country.
Company names, products/service names and logos used in this publication are trademarks and trade names of Shimadzu Corporation, its subsidiaries or its affiliates, whether or not they are used with trademark symbol "TM" or "®".
Third-party trademarks and trade names may be used in this publication to refer to either the entities or their products/services, whether or not they are used with trademark symbol "TM" or "®".
Shimadzu disclaims any proprietary interest in trademarks and trade names other than its own.

The contents of this publication are provided to you "as is" without warranty of any kind, and are subject to change without notice.
Shimadzu does not assume any responsibility or liability for any damage, whether direct or indirect, relating to the use of this publication.

© Shimadzu Corporation, 2022 / First Edition: June 2022, 3655-06205-PDFIK, C146-E462