

Quadrupole Time-of-Flight Liquid Chromatograph Mass Spectrometer

LCMS-9030



Effortless Performance

The LCMS-9030 quadrupole time-of-flight (QTOF) 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.

LCMS-9030

Quadrupole Time-of-Flight Liquid Chromatograph Mass Spectrometer

Greater **Accuracy**

Better **Sensitivity**

Higher **Resolution**

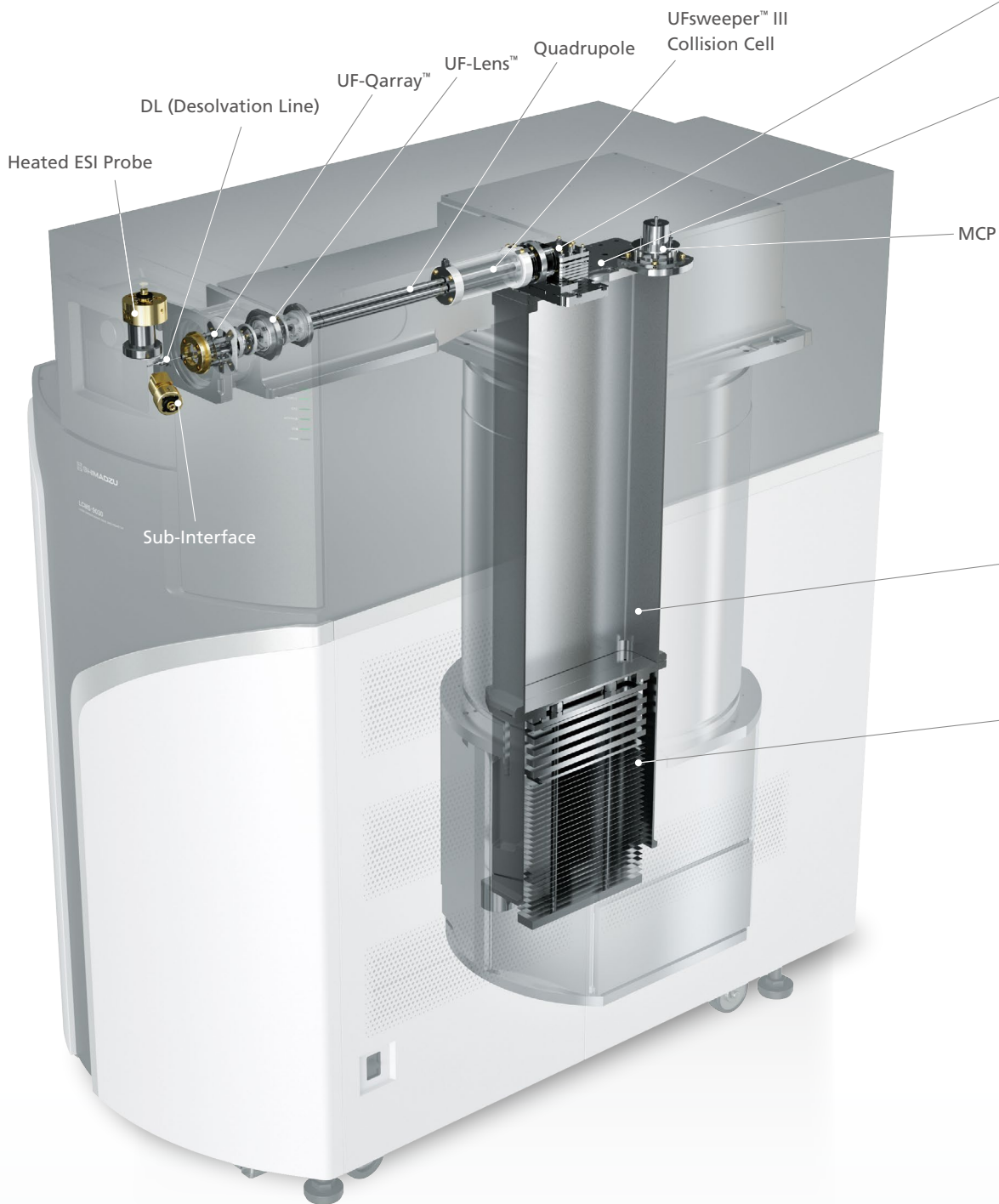


Key Technologies of the LCMS-9030

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



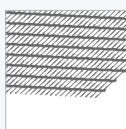
» New TOF Technologies

UFaccumulation™ (Pat. US 10020181)

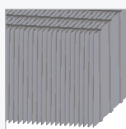
Ion accumulation in the collision cell, synchronized perfectly with short cycles of data acquisition, maximizes sensitivity.

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.



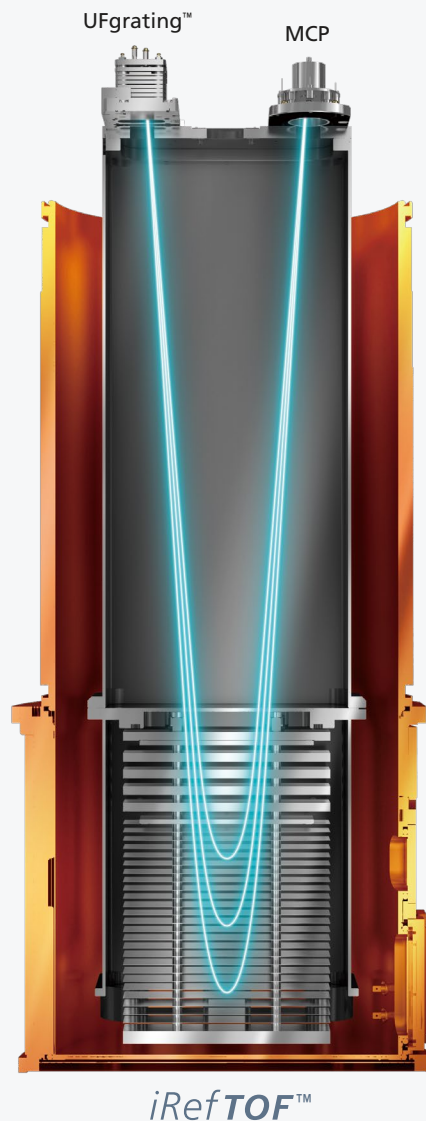
Shimadzu's UFgrating has superior mechanical strength over conventional electrodes. This unique grating structure makes it possible to apply a higher voltage.

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.



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)

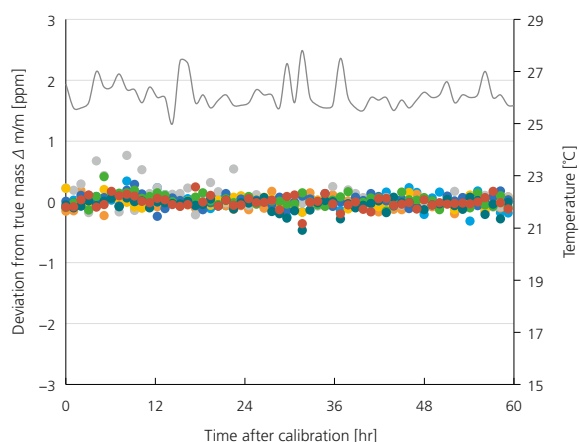
Stable MMA Against Temperature Fluctuation

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.

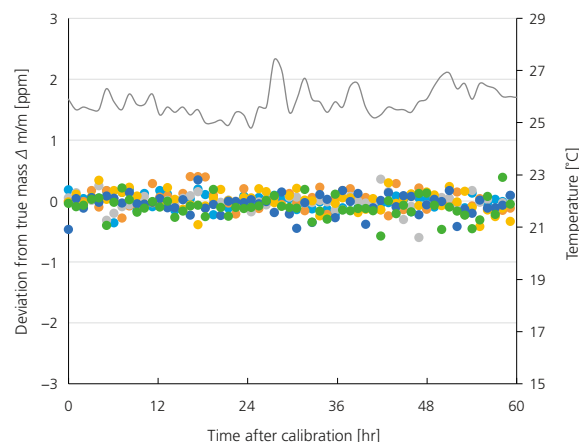
With the LCMS-9030, laboratory productivity can be increased by running long, calibration-free batches with confidence.

Positive Mode



- Acetoaminophen
- Anisomycin
- Progesterone
- Mitomycin C
- Griseofulvin
- Doxorubicin
- Rifampicin
- Valinomycin
- Temperature

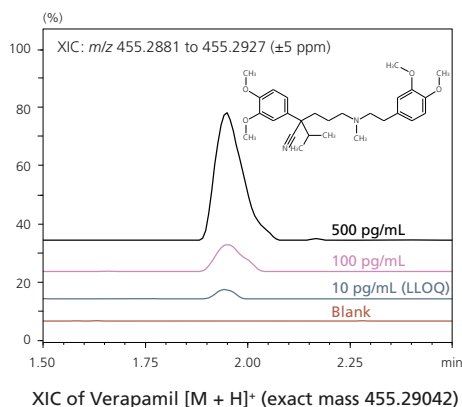
Negative Mode



- Doxorubicin
- Salinomycin
- Thiostrepton
- Tubercidin
- Valinomycin
- Mitomycin C
- Temperature

High MMA Over Wide Concentrations

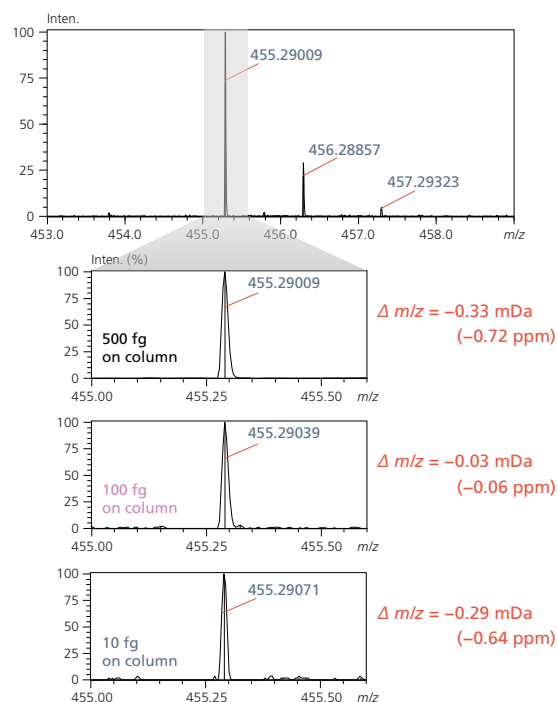
The LCMS-9030 breaks new ground for quantitative analysis not only by its high sensitivity but also by the selectivity afforded by high MMA over a wide range of concentrations. Genuine ion statistics ensure that all measurements throughout the peak elution result within a narrow m/z window of the extracted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



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 |

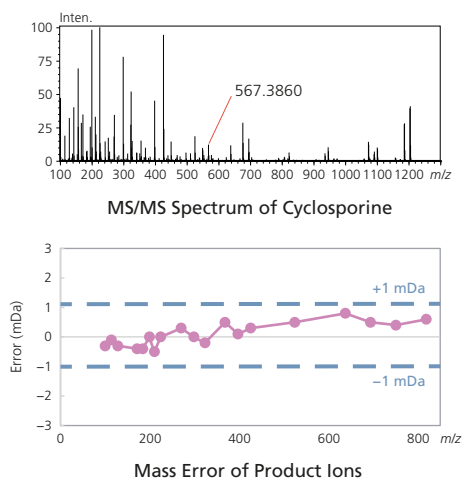
was less than 1 ppm and all data points gave results within the 5 ppm XIC window for accurate, repeatable and selective quantitation. Moreover, stability of MMA allows the same XIC setting to be comfortably used for series of analyses.



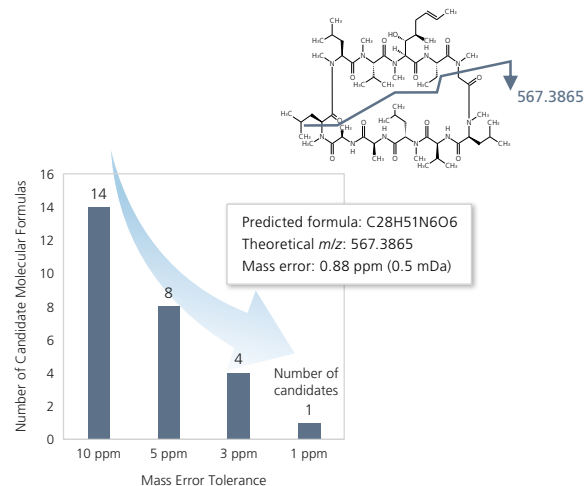
Averaged Mass Spectrum at Each Concentration

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.

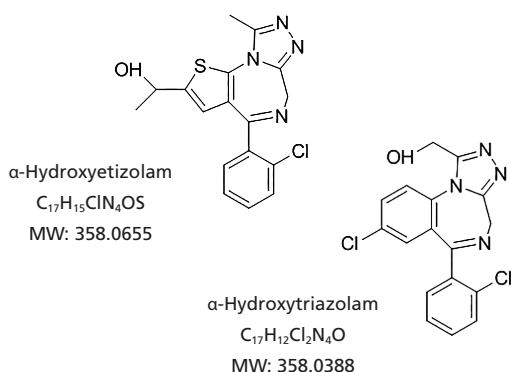


The results of MS/MS structural analysis of cyclosporine are shown below. Numerous ions were matched with putative fragment structures at less than 1 mDa mass error. Formula prediction results for m/z 567.3860 at different mass error tolerances demonstrate the impact of MS/MS MMA in making the prediction unambiguous.

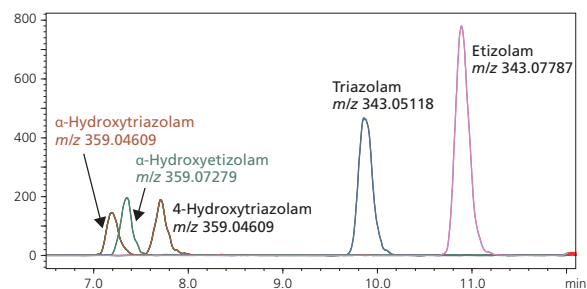


HRAM for Selective Detection of Isobaric Compounds

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.

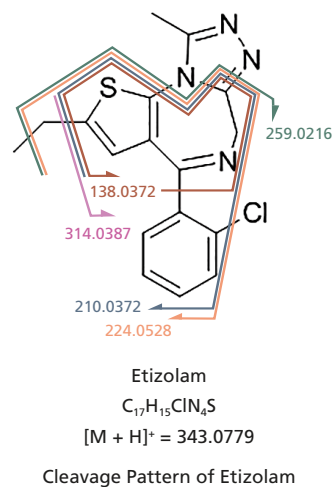
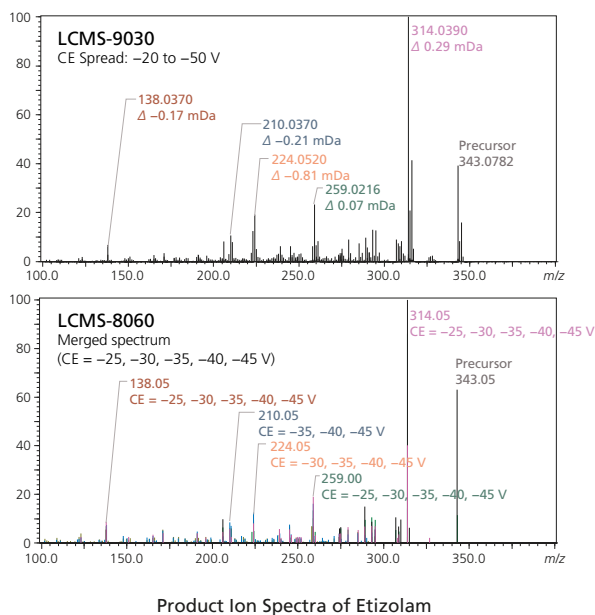


LCMS-9030 Mass Chromatogram of Etizolam, Triazolam, and Metabolites Spiked at 10 ng/mL in Whole Blood.

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 QTOF 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 QTOF DDA experiments.



Data Courtesy of Associate Professor Kei Zaitzu (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)



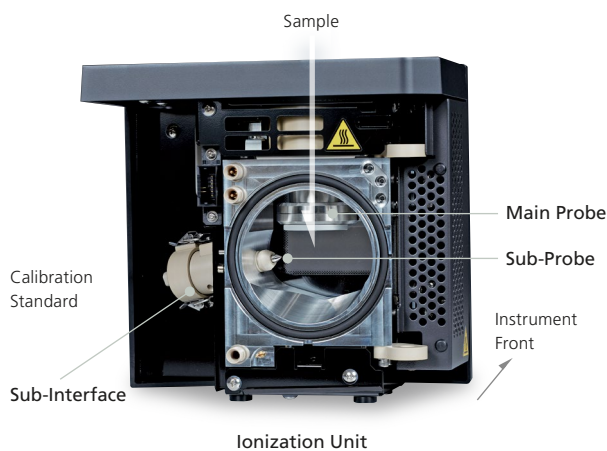
DUIS™ (optional)

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



Calibrant Delivery System (CDS)

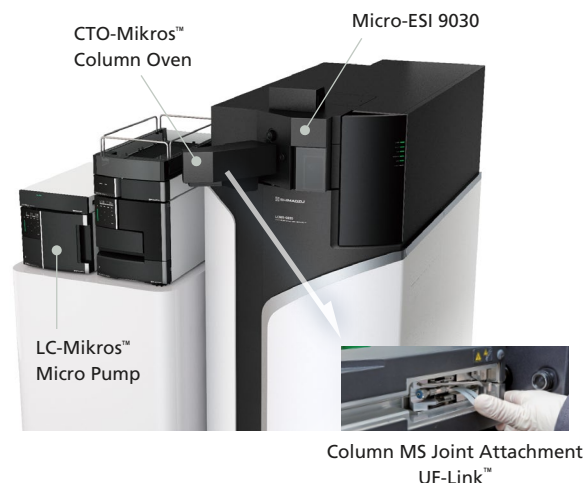
The CDS allows calibration standards to be introduced via a separate ionization probe that functions independently from the main probe. This optional sub-ionization unit is installed in the main probe housing and is available for all probe types (ESI/APCI/DUIS). By having two probes in one system, high-concentration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



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 QTOF. 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 Supporting both Qualitative and Quantitative Analysis

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.

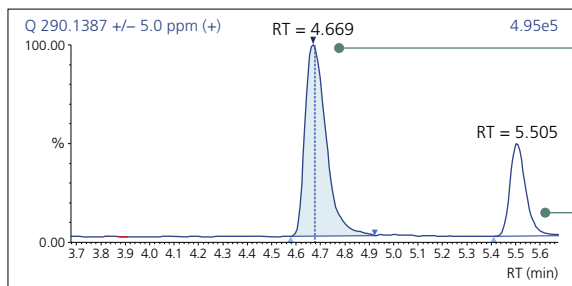
The screenshot displays the LabSolutions Insight Explore software interface. Key components are labeled as follows:

- Sample List:** A table listing sample details such as Sample No., Run, Sample Type, and Cut Point.
- Compound Results:** A table showing the results of the analysis, including Name, Retention Time (Ret. Time), and other parameters.
- List of MS Chromatogram:** A plot showing the chromatogram for a specific sample, with peaks labeled by their retention times.
- List of MS Spectrum:** A plot showing the mass spectrum for a specific peak, with the base peak at m/z 290.1387.
- Assign, Analyze, Formula Calculator:** A section for structural analysis, showing the chemical structure of Benzoylgonine and its molecular formula $C_{16}H_{19}NO_4$.

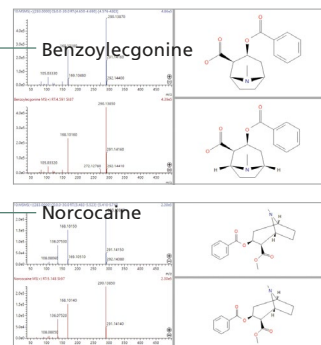
Structural Analysis Function: "Assign"

Compounds with the same molecular formulae cannot be distinguished by their mass peaks even using an instrument with high mass precision. But with the "Assign" structural analysis function, combined with the library search function, it becomes possible to identify these compounds with great accuracy. Below is an example analysis of Benzoylgonine and Norcocaine, two compounds with the same molecular formula of $C_{16}H_{19}NO_4$ (m/z : 290.1387).

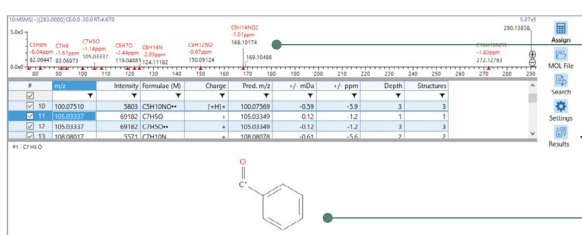
MS Chromatogram (m/z : 290.1387)



Library Search Results



Structural Analysis Results for Benzoylgonine



Compound Search Function: "Analyze"

Using the "Analyze" compound search function, elucidate the composition of unknown compounds from precise MS data and look up their molecular and structural formulae.

Search for Candidates

| RT (m/z) | Response | Width | RT Group | Predict | Predicted Formula | Ito Score |
|------------|-----------|---------|----------|---------|-------------------------------|-----------|
| 301 8.820 | 313.23894 | 814350 | 0.187 | 132 | [C18 H28 O4 H] ⁺ | 94.55 |
| 303 9.123 | 303.23185 | 6980606 | 0.333 | 134 | [C20 H30 O2 H] ⁺ | 67.90 |
| 305 9.383 | 303.21650 | 6130963 | 0.300 | 135 | [C20 H30 O2 H] ⁺ | 76.85 |
| 312 10.397 | 303.23180 | 4979776 | 0.273 | 139 | [C20 H30 O2 H] ⁺ | 55.56 |
| 319 5.977 | 324.20692 | 5404965 | 0.353 | 144 | [C20 H25 N O H] ⁺ | 76.18 |
| 322 6.593 | 322.17997 | 2424747 | 0.433 | 145 | [C21 H25 N O2 H] ⁺ | 75.81 |
| 324 6.624 | 327.15688 | 3198090 | 0.453 | 146 | [C18 H19 N C H] ⁺ | 98.60 |

Narrow Down the Candidates

| RT (m/z) | Response | Width | RT Group | Predict | Predicted Formula | Ito Score |
|------------|-----------|---------|----------|---------|-------------------------------|-----------|
| 301 8.820 | 313.23894 | 814350 | 0.187 | 132 | [C18 H28 O4 H] ⁺ | 94.55 |
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Process the Search Results with the "Assign" Function

| Name | Formula | Mass | Charge | Peak (m/z) | Delta | Structure |
|------|----------|----------|--------|------------|-------|-------------------------------|
| 1 | C20H30O2 | 302.2318 | + | 303 | 0.75 | <chem>CCCCCCCCCCCCCCCC</chem> |
| 2 | C20H25NO | 303.1962 | + | 304 | 0.75 | <chem>CCCCCCCCCCCCCCCC</chem> |
| 3 | C20H25NO | 303.1962 | + | 304 | 0.75 | <chem>CCCCCCCCCCCCCCCC</chem> |

Search with PubChem®/ChemSpider

MOL Search

PubChem ChemSpider

Formula: C22 H28 N2 O

Mass: 336.22016 +/- ppm 5

Sort: None

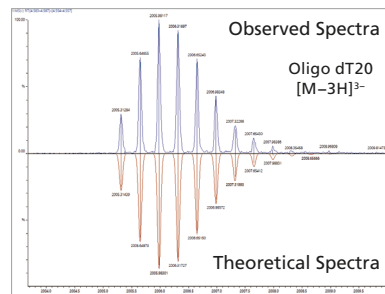
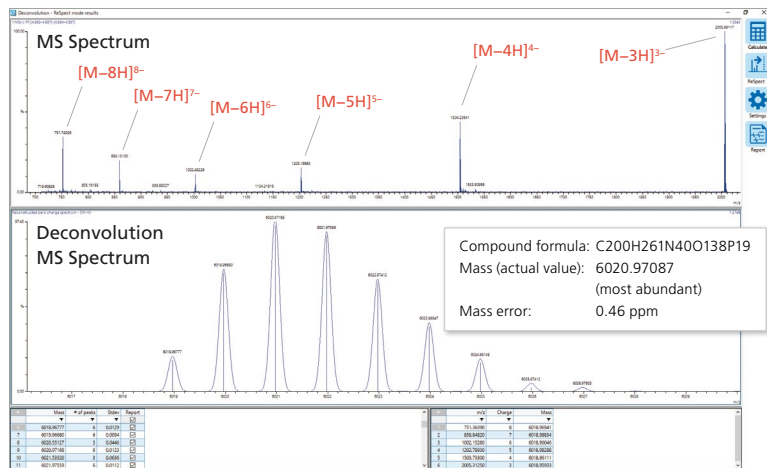
Max Results: 20

Order By: #PubMed

Auto Assign

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 related multi-charged peaks and calculates the mass of the original species. Excellent mass accuracy was obtained in the example below.



Comparison of Observed and Theoretical Spectra

Deconvolution Example (Oligo dT20)

UF-Qarray, UF-Lens, UFsweeper, UFaccumulation, UFgrating, UF-FlightTube, iRefTOF, DUIS, UF-Link, Nexera Mikros, CTO-Mikros, LC-Mikros and LabSolutions Insight Explore are trademarks of Shimadzu Corporation or its affiliated companies in Japan and/or other countries.
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