C146-E462B

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 QTOF 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**

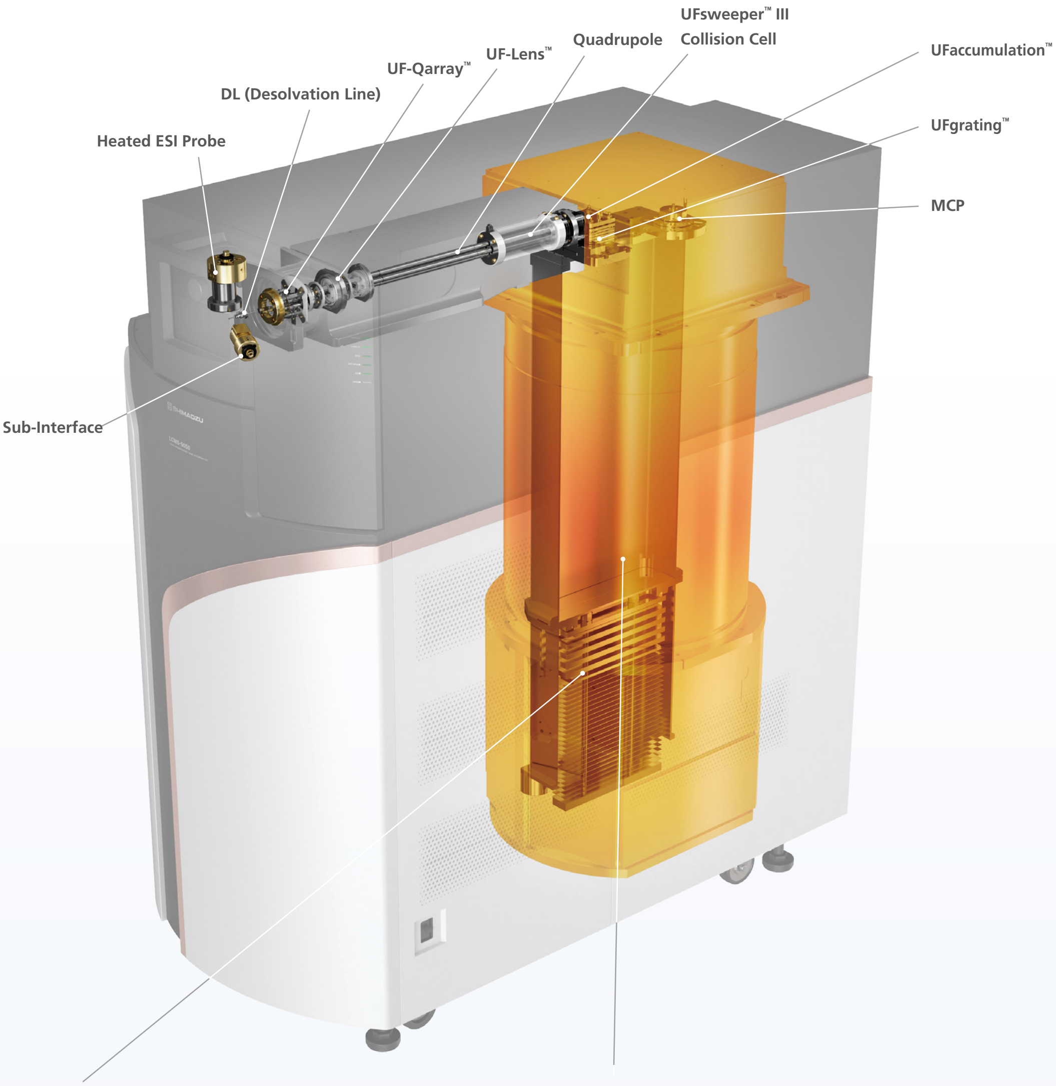
Truly versatile with **flexible extensions**


POWER
STATUS
GAS
INTERFACE
CDS
ERROR
SHIMADZU
LCMS-9050
LIQUID CHROMATOGRAPH MASS SPECTROMETER

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



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

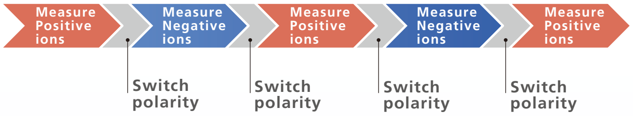
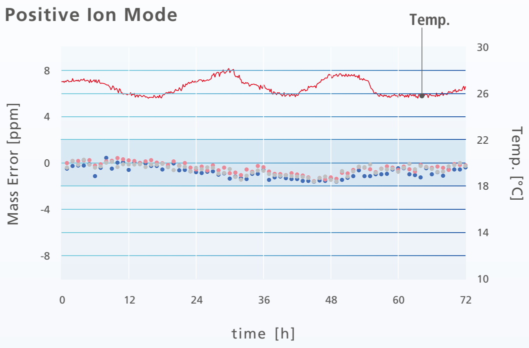
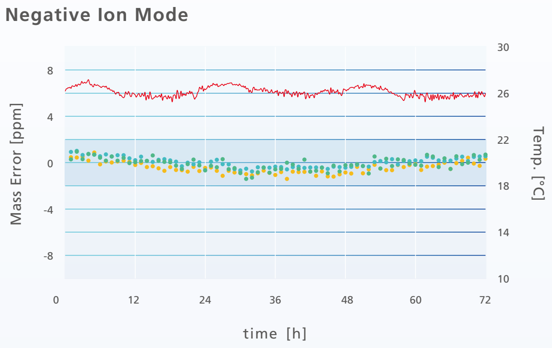
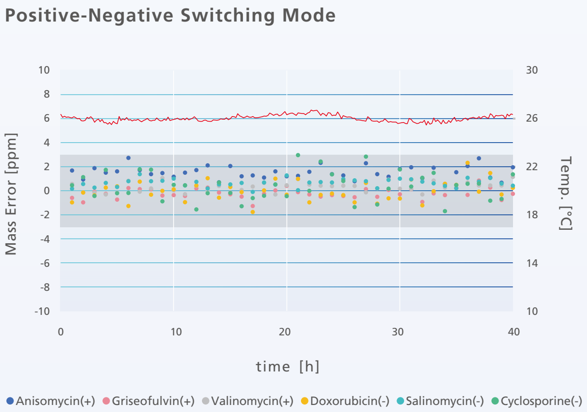


Illustration of Switching between Positive and Negative Ion Modes

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


Positive Ion Mode


Negative Ion Mode


Positive-Negative Switching Mode

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.

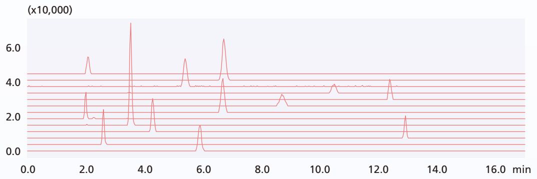
Results of analyzed 6 antibioticcomponents continuously

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.*

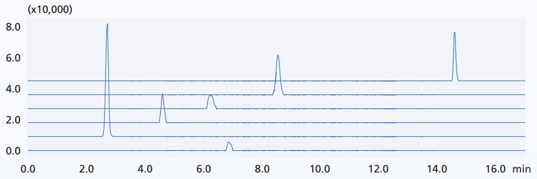
Increasing Workflow Efficiency with Polarity Switching

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

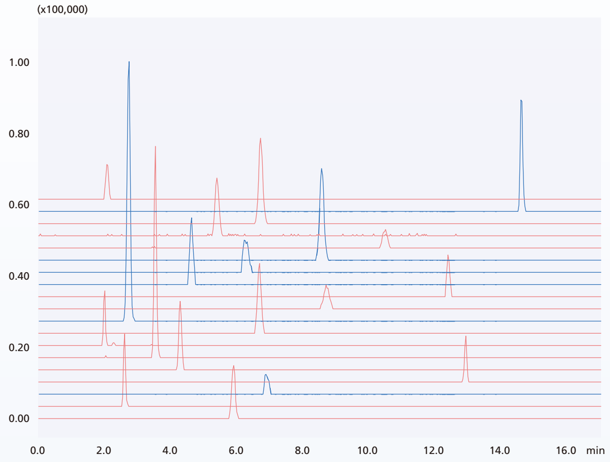


Negative Ion Mode Measurement

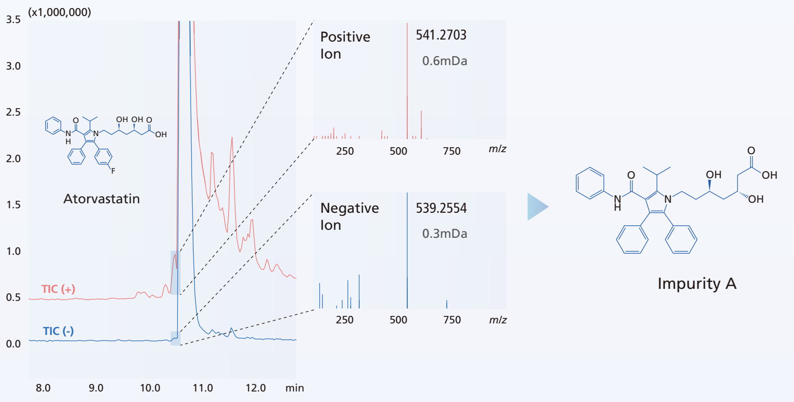


Conventional QTOF

Positive-Negative Switching Mode Measurement



LCMS-9050



Impurity Analysis of Atorvastatin

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.

* The specified mass accuracy may not be achieved depending on analytical conditions.

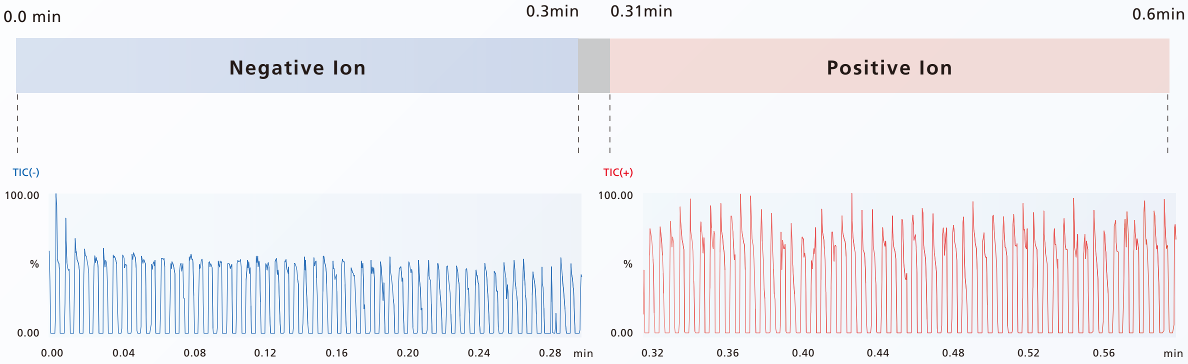
Truly versatile with flexible extensions

A wide variety of analytical challenges can be further addressed by combining the QTOF 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.

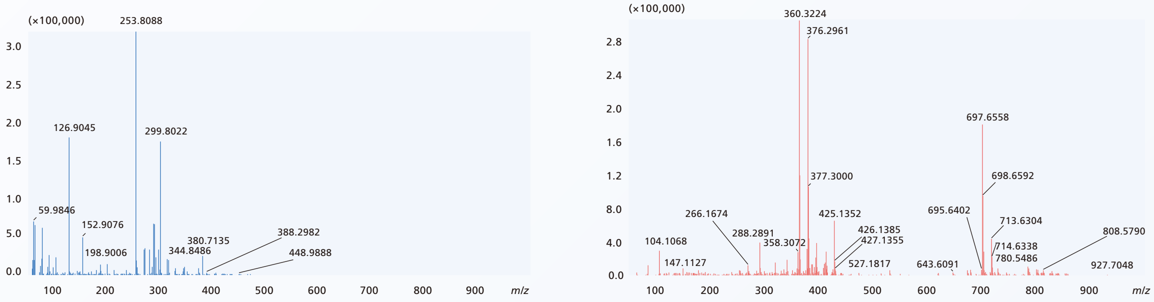
DPiMS™

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 QTOF, 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 QTOF 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, QTOF is the best combination for this purpose.

OAD RADICAL SOURCE I

Oxygen Attachment Dissociation MS/MS Option Kit

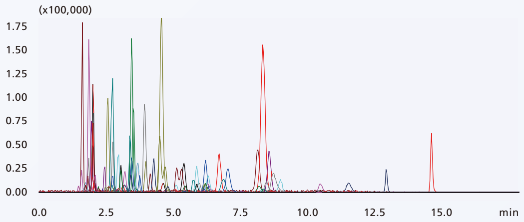
OAD RADICAL SOURCE I is an optional product for Shimadzu QTOF systems that enables oxygen attachment dissociation (OAD), Shimadzu’s proprietary fragmentation method. It allows the analysis of the position of carbon-to-carbon double bonds in lipids and other organic compounds.

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 QTOF, the system is powerful for full screening of multiple components.



80 components of pesticides Mass Chromatogram

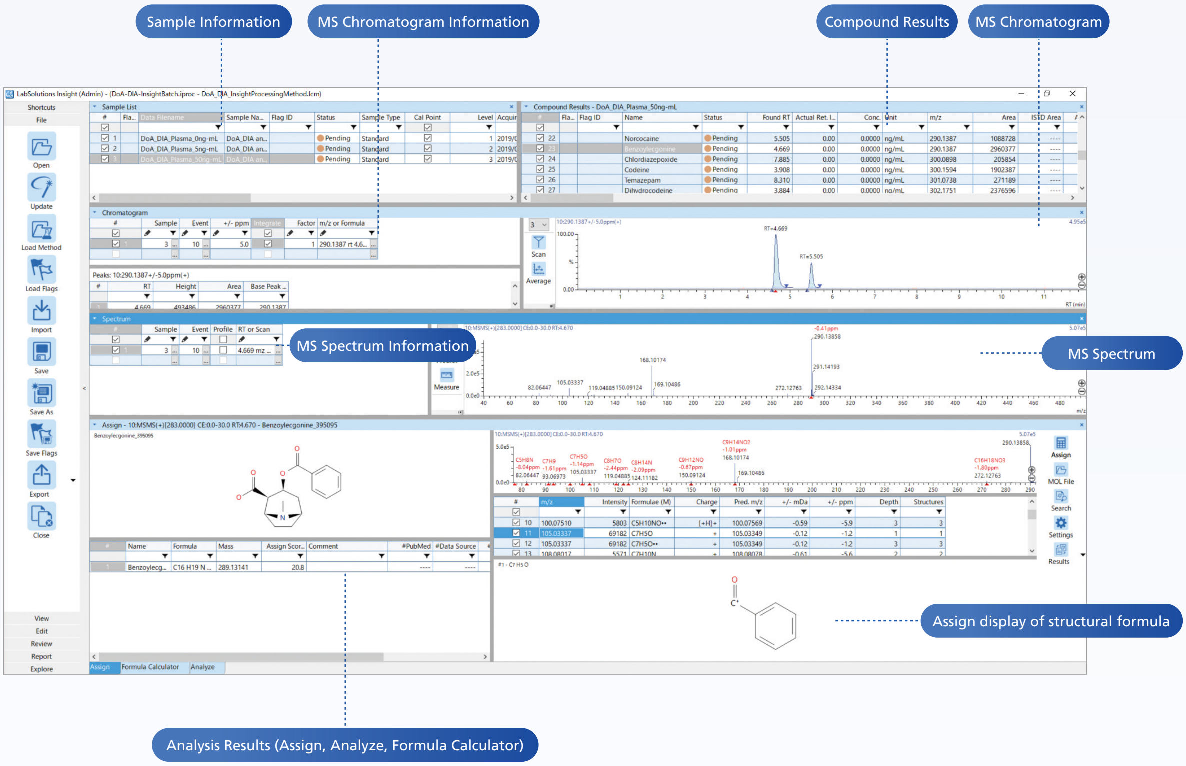
Nexera Mikros™

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 QTOF 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.



LabSolutions Insight (Admin) - (DoA-DIA-InsightBatch.iproc - DoA_DIA_InsightProcessingMethod.lcm)

Sample List

#	Fla...	Data Filename	Sample Na...	Flag ID	Status	Sample Type	Cal Point	Level	Acquir
☑ 1		DoA_DIA_Plasma_0ng-mL	DoA_DIA an...		Pending	Standard	☑	1	2019/(
☑ 2		DoA_DIA_Plasma_5ng-mL	DoA_DIA an...		Pending	Standard	☑	2	2019/(
☑ 3		DoA_DIA_Plasma_50ng-mL	DoA_DIA an...		Pending	Standard	☑	3	2019/(

Compound Results - DoA_DIA_Plasma_50ng-mL

#	Fla...	Flag ID	Name	Status	Found RT	Actual Ret. I...	Conc.	Unit	m/z	Area	ISTD Area
☑ 22			Norcocaine	Pending	5.505	0.00	0.0000	ng/mL	290.1387	1088728	----
☑ 23			Benzoylecgonine	Pending	4.669	0.00	0.0000	ng/mL	290.1387	2960377	----
☑ 24			Chlordiazepoxide	Pending	7.885	0.00	0.0000	ng/mL	300.0898	205854	----
☑ 25			Codeine	Pending	3.908	0.00	0.0000	ng/mL	300.1594	1902387	----
☑ 26			Temazepam	Pending	8.310	0.00	0.0000	ng/mL	301.0738	271189	----
☑ 27			Dihydrocodeine	Pending	3.884	0.00	0.0000	ng/mL	302.1751	2376596	----

Chromatogram

#	Sample	Event	+/- ppm	Integrate	Factor	m/z or Formula
☑ 1	3	10	5.0	☑	1	290.1387 rt 4.6...

10:290.1387+/-5.0ppm(+)

Peaks: 10:290.1387+/-5.0ppm(+)

#	RT	Height	Area	Base Peak ...
1	4.669	493486	2960377	290.1387

Spectrum

#	Sample	Event	Profile	RT or Scan
☑ 1	3	10	☐	4.669 mz ...

10:MSMS(+)[283.0000] CE:0.0-30.0 RT:4.670

Assign - 10:MSMS(+)[283.0000] CE:0.0-30.0 RT:4.670 - Benzoylecgonine_395095

Benzoylecgonine_395095

#	Name	Formula	Mass	Assign Scor...	Comment	#PubMed	#Data Source
1	Benzoylecg...	C16 H19 N ...	289.13141	20.8		----	----

#	m/z	Intensity	Formulae (M)	Charge	Pred. m/z	+/- mDa	+/- ppm	Depth	Structures
☑ 10	100.07510	5803	C5H10NO••	[+H]+	100.07569	-0.59	-5.9	3	3
☑ 11	105.03337	69182	C7H5O	+	105.03349	-0.12	-1.2	1	1
☑ 12	105.03337	69182	C7H5O••	+	105.03349	-0.12	-1.2	3	3
☑ 13	108.08017	5571	C7H10N	+	108.08078	-0.61	-5.6	2	2

#1 - C7 H5 O

Assign | Formula Calculator | Analyze

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) indudes "*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.
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