

Liquid Chromatograph Mass Spectrometer

# LCMS-8045

*UFMS*  
ULTRA FAST MASS SPECTROMETRY



# UPLC

ULTRA FAST MASS SPECTROMETRY

## Speed Beyond Comparison

# LCMS-8045

—*Best-in-class sensitivity*

### ■ Accomplishes Both High Sensitivity and Ultra-High-Speed Detection

Equipped with a heated ESI probe, the LCMS-8045 has the highest\* sensitivity in its class. The instrument is capable of providing accurate and stable data over long periods of time. The inclusion of Shimadzu's ultra-high-speed high-voltage power supply enables the world's fastest\* scan speed (30,000 u/s) and polarity switching time (5 ms). High-speed acquisition benefits the laboratory by reducing run times for increased throughput, and also shortens method development time.

\* As of August 2016, according to a Shimadzu survey

### ■ Superior Robustness Assures That High Sensitivity Is Maintained Over the Long Term

The LCMS-8045 was designed to be robust. The heated ESI probe, high-temperature heating block, heated desolvation line, drying gas, and focusing optics all act to maximize sensitivity and minimize contamination. This means long periods of continuous operation in the laboratory with reliable data collection, even with complex biological fluids or food samples.

### ■ LabSolutions™ LCMS Software and Wide-Ranging Method Packages

LabSolutions LCMS features an intuitive user interface, and offers the latest features designed to enhance laboratory productivity and streamline workflows. Numerous pre-configured MRM method packages are available. Predetermined LC separation conditions and MRM parameters allow analysis to be started without long hours of method development, enhancing the efficiency of your laboratory.

### ■ Heated ESI Probe

High-temperature gas supplements the nebulizer gas, improving desolvation efficiency. This facilitates the ionization of a wide range of compounds.

### ■ Ultrafast High-Voltage Power Supply for Polarity Switching



### ■ Ionization Unit

Designed without cables or tubes; utilize a one-touch lever to perform simple attachment and detachment of the unit.

### ■ DL (Desolvation Line)

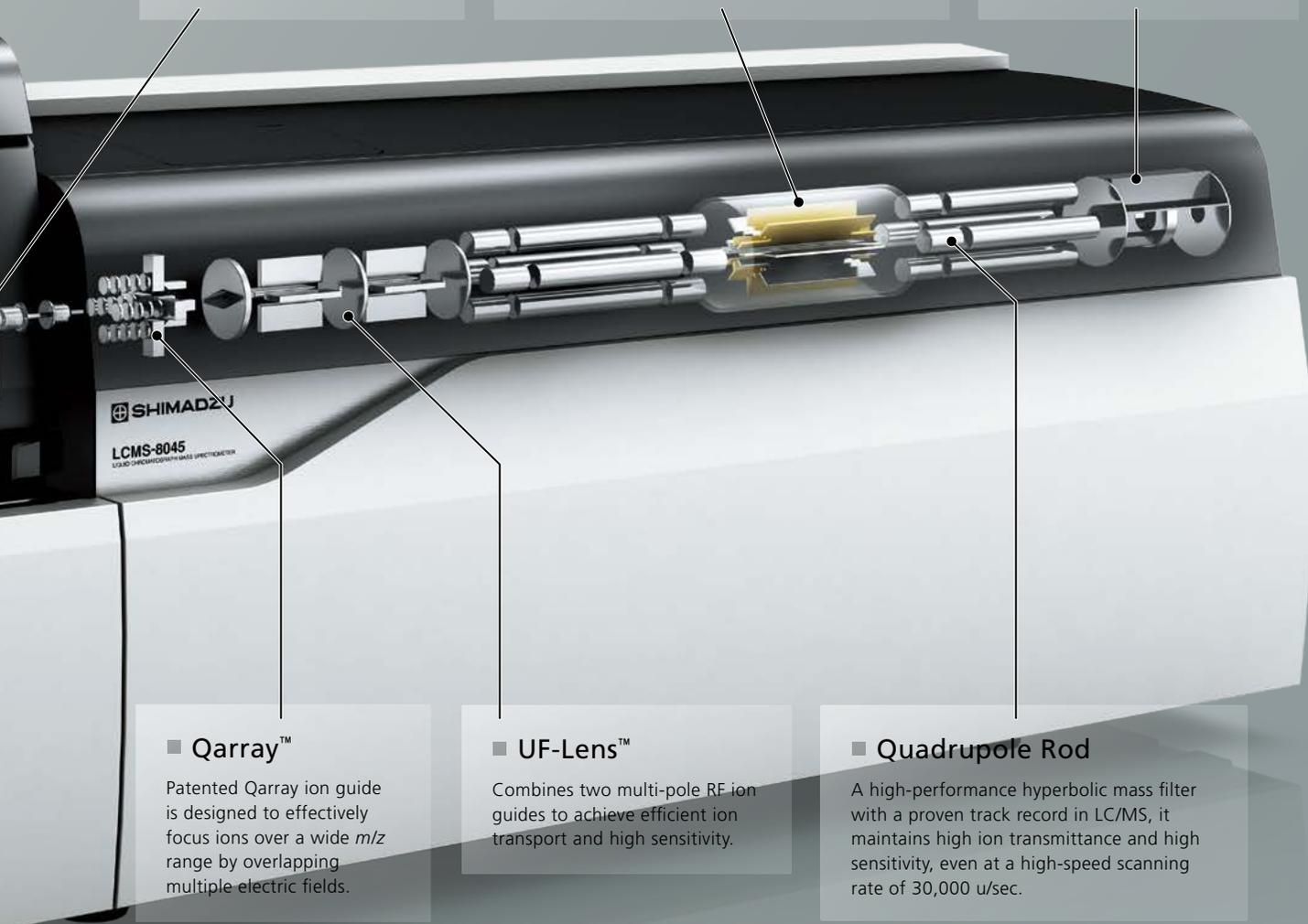
Perform maintenance without breaking vacuum.

### ■ UFsweeper™ II Collision Cell

The UFsweeper II is a high-sensitivity, high-speed collision cell that features improved ion focusing by using high-speed ion transport technology. This yields better product ion transmission in the collision cell, maintaining signal intensity and suppressing crosstalk, even for high-speed or simultaneous multi-component analysis. The capability for high-throughput analysis is thus maintained at lower levels of detection.

### ■ Ultrafast Pulse-Counting Detector

Makes ultrafast sampling and polarity switching possible.



### ■ Qarray™

Patented Qarray ion guide is designed to effectively focus ions over a wide  $m/z$  range by overlapping multiple electric fields.

### ■ UF-Lens™

Combines two multi-pole RF ion guides to achieve efficient ion transport and high sensitivity.

### ■ Quadrupole Rod

A high-performance hyperbolic mass filter with a proven track record in LC/MS, it maintains high ion transmittance and high sensitivity, even at a high-speed scanning rate of 30,000  $u/sec$ .

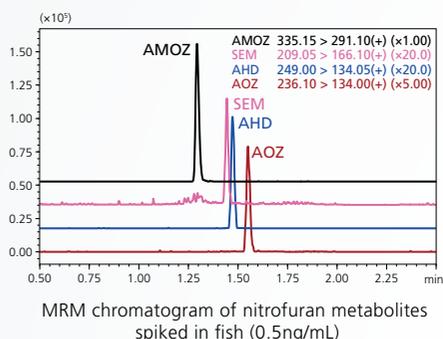
# High Performance for a Variety of Applications

## Veterinary Drugs

### ■ Nitrofuran metabolites in fish

Nitrofurans are a class of synthetic antibiotics. The use of nitrofurans for edible animal and fishery products is banned in many countries. The chromatogram below shows the recovery of nitrofuran metabolites from fish using the LCMS-8045. Excellent linearity and accurate quantitative

results ranging from 0.05 to 20 ng/mL were obtained. The LCMS-8045 is shown to be an excellent platform for routine high-sensitivity analysis in challenging matrices.



Calibration range, accuracy and limit of detection (LOD)

Compound	Calibration range (ng/mL)	Accuracy (%)	LOD (ng/mL)
AMOZ	0.05 – 20	94.5 – 103.8	0.00024
SEM	0.05 – 20	93.2 – 111.6	0.015
AHD	0.05 – 20	95.5 – 102.1	0.001
AOZ	0.05 – 20	94.0 – 108.4	0.00096

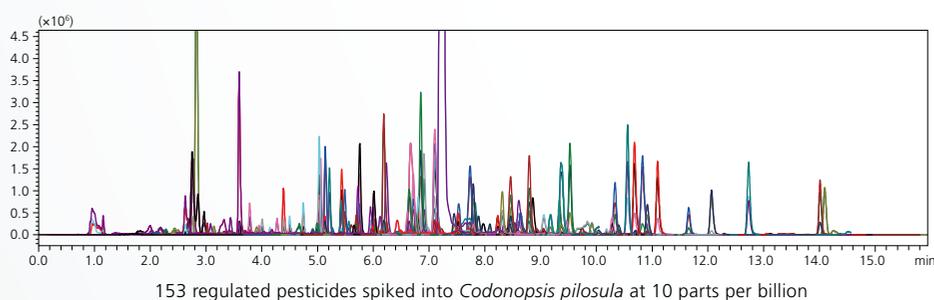
\* Limit of detection (LOD) was calculated at signal-to-noise ratio (S/N) = 3.

## Residual Pesticides

### ■ Simultaneous analysis of residual pesticides in herbal supplements

Regulatory agencies worldwide provide oversight for an extensive and ever-increasing list of pesticides in order to promote food safety and protect public health. The MRM chromatogram below shows the simultaneous analysis of 153 pesticides spiked into *Codonopsis pilosula* at 0.01 mg/kg. Plant matrices can be very challenging due to background

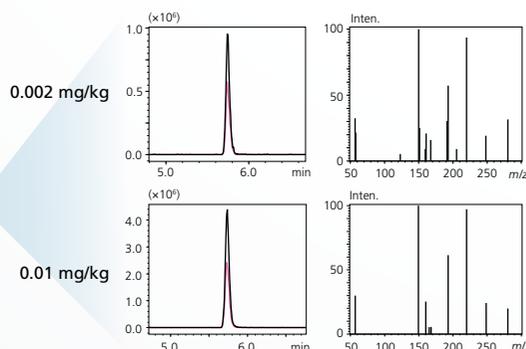
interferences, but the LCMS-8045 provides enough sensitivity to analyze most pesticides at the trace level of 10 parts per billion. Many pesticides methods also benefit from polarity switching, which the LCMS-8045 can accomplish in just 5 msec.



Use Synchronized Survey Scan™ (SSS) to obtain both qualitative and quantitative information from a single injection. Full scan MS<sup>2</sup> spectra will be obtained when an MRM peak intensity threshold is exceeded.

Type	Event#	+/-	Compound Name m/z	Time (0.000 min – 15.939 min)
MRM	63	±	Metalaxyl 280.10>220.20, 2	
Product Ion Scan	64	+	> CE: -18.0, 50.00:300.00	
MRM	65	+	Atrazine 216.10>174.05, 2	
Product Ion Scan	66	+	> CE: -20.0, 50.00:250.00	
MRM	67	+	Fensulfotoin-sulfone 324	
Product Ion Scan	68	+	> CE: -28.0, 50.00:350.00	
MRM	69	+	N-desethyl-pirimphos-me	
Product Ion Scan	70	+	> CE: -25.0, 50.00:300.00	

Method settings and Synchronized Survey Scan results for Metalaxyl



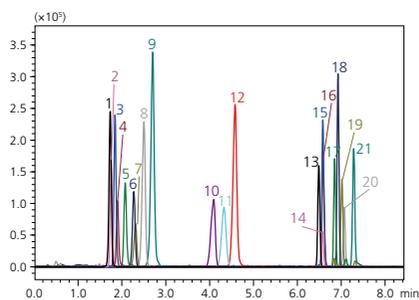
## Water Quality Analysis



### High-sensitivity analysis of 21 pharmaceuticals and personal care products in less than eight minutes

Pharmaceutical and personal care products (PPCPs) encompass a family of compounds used by individuals for health and cosmetic purposes. As populations increase, and the use of these products increases, PPCPs will

become a significant threat to our water supply. The LCMS-8045 is capable of trace-level quantitation of many PPCPs without extensive sample preparation.



MRM chromatograms of 21 PPCPs (1.0 ng/mL)

The limit of detection (LOD) and limit of quantitation (LOQ) for 21 PPCPs

No.	Compound	LOD (ng/mL)	LOQ (ng/mL)	No.	Compound	LOD (ng/mL)	LOQ (ng/mL)	No.	Compound	LOD (ng/mL)	LOQ (ng/mL)
1	Lincomycin	0.01	0.04	8	Metoprolol	0.013	0.04	15	Clarithromycin	0.0034	0.01
2	Trimethoprim	0.01	0.04	9	Dicorantil	0.005	0.015	16	Roxithromycin	0.0071	0.022
3	Pirenzepine	0.01	0.03	10	Sulfamethoxazole	0.003	0.01	17	Carbamazepine	0.01	0.03
4	Ofloxacin	0.01	0.03	11	Antipyrine	0.01	0.03	18	DEET	0.0062	0.018
5	Ciprofloxacin	0.002	0.006	12	Ifenprodil	0.0075	0.022	19	Crotamiton	0.005	0.015
6	Sulphapyridine	0.002	0.006	13	Erythromycin	0.015	0.045	20	Bezafibrate	0.0025	0.075
7	Carbazochrome	0.015	0.045	14	Azithromycin	0.01	0.03	21	Triclocarban	0.01	0.03

\* Limit of detection (LOD) was calculated at signal-to-noise ratio (S/N) = 3. Limit of quantitation (LOQ) was calculated at S/N = 10.

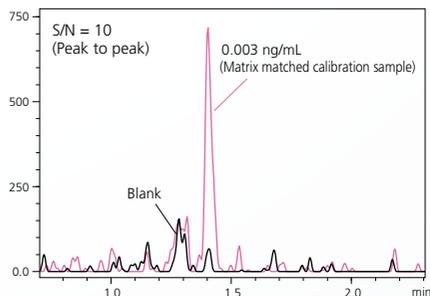
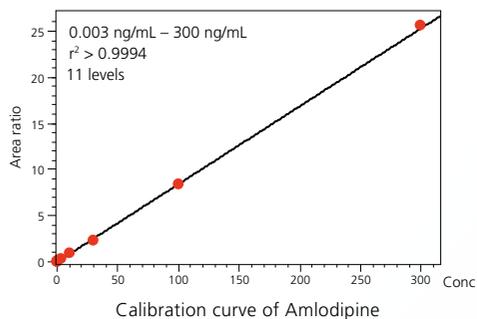
## Bioanalysis



### High-sensitivity quantitation of Amlodipine in plasma

Amlodipine is widely utilized for the treatment of high blood pressure and angina. A high-sensitivity method for the quantitation of amlodipine in human plasma using LCMS-8045 has been developed. Appropriate linearity ranging from 0.003 to 300 ng/mL with excellent accuracy was

achieved. Both interday and intraday variabilities were assessed for quality control samples. Percent RSD (Relative Standard Deviation) results were less than 5%.



MRM chromatogram of Amlodipine at the lower limit of quantitation  
Black: Blank, Pink: Matrix matched calibration sample (0.003 ng/mL)

Quantitative results of Amlodipine

Lv	Actual conc. (ng/mL)	Calculated Conc. (ng/mL)	Accuracy (%)
1	0.003	0.003	104.5
2	0.01	0.01	97.2
3	0.03	0.031	103
4	0.1	0.107	107.1
5	0.3	0.268	89.4
6	1	1.062	106.2
7	3	2.958	98.6
8	10	10.293	102.9
9	30	27.37	91.2
10	100	98.722	98.7
11	300	303.619	101.2

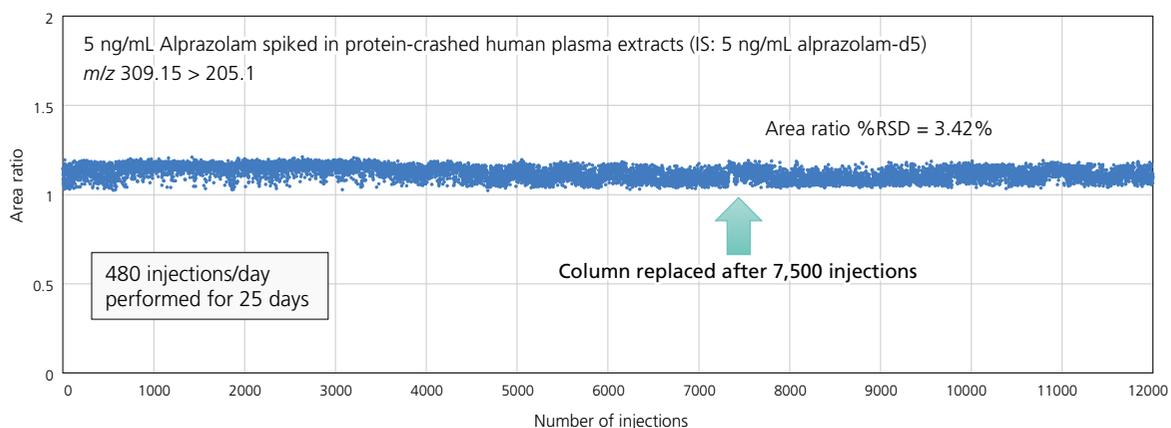
Interday and intraday variations of Amlodipine spiked in human plasma

QC sample	Concentration (ng/mL)	%RSD	Accuracy (%)
Interday Variation (n = 6)	Low	0.1	3.78
	Medium	5	3.16
	High	240	0.85
Intraday Variation (n = 18)	Low	0.1	4.5
	Medium	5	4.92
	High	240	4.25

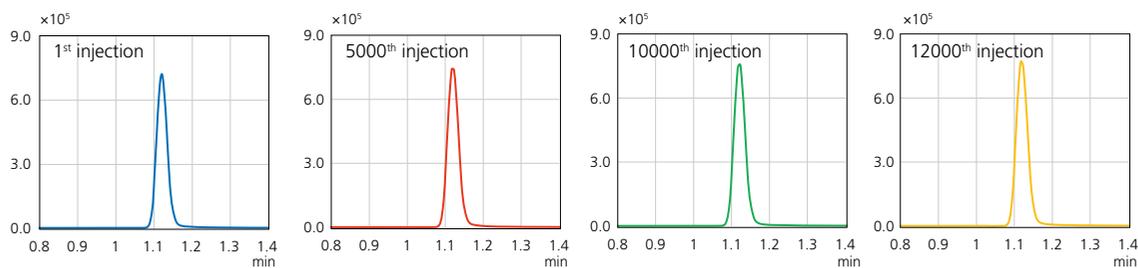
# Consistent High-Sensitivity Performance

## ■ Robust Ion Source and Sample Introduction System

Shimadzu's MS interface includes a high-sensitivity heated ESI source, heated capillary sample introduction, and proprietary ion transfer optics. These design features combine to produce robust MS performance. 12,000 plasma samples were injected over 25 days (over 480 samples per day). Picogram levels of alprazolam were analyzed with an RSD of 3.42%.



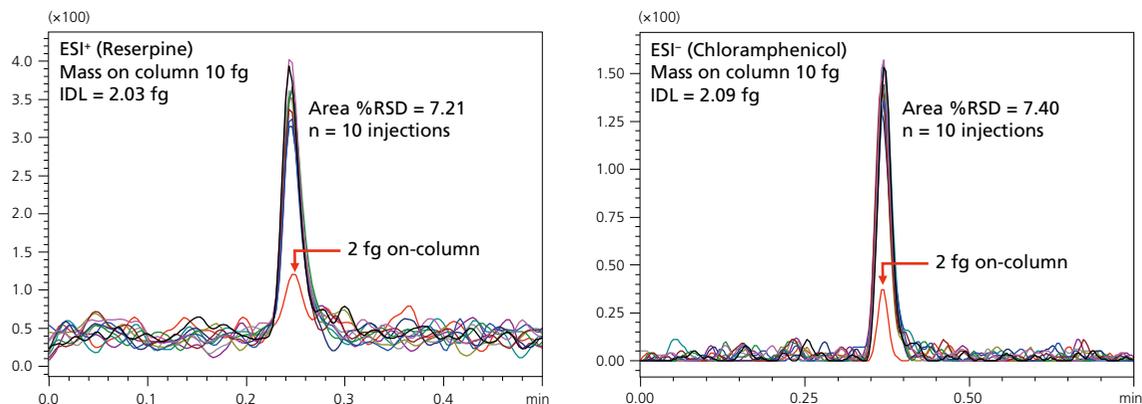
LCMS-8045 Instrument Stability Test



MRM Chromatograms of Alprazolam

## ■ Instrument Detection Limits: IDL

IDL is one measure of sensitivity for analytical instrumentation. The chromatograms below show the IDL for Reserpine and Chloramphenicol, obtained using ESI<sup>+</sup> and ESI<sup>-</sup>, respectively. The IDL for Reserpine is 2.03 femtograms and 2.09 femtograms for Chloramphenicol.



## ■ Newly Designed Ionization Unit

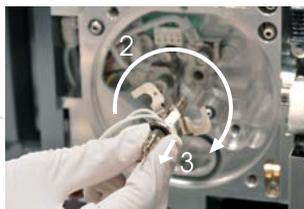
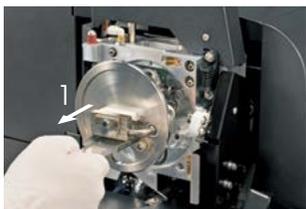
Designed without cables or tubes, removing the new ionization unit is simple: release a one-touch lever to open the unit and lift it out. In addition, no tools are needed to detach the needles fitted in APCI and DUIS™ units, allowing for easy maintenance.



## ■ Easy System Maintenance Reduces Downtime

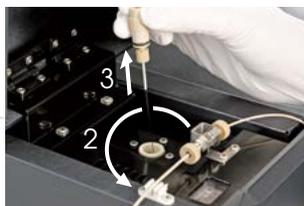
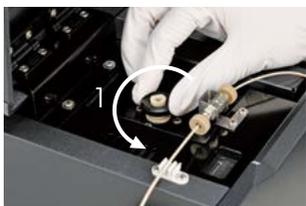
As with Shimadzu's other triple quad systems, maintaining the LCMS-8045 is simple. Replacing the desolvation line (DL) and ESI capillary is quick and easy. Additionally, the design allows users to replace the DL without breaking vacuum, providing greater uptime and usability.

### ● Steps for DL Replacement



DL (Desolvation Line)

### ● Steps for ESI Capillary Replacement



ESI Capillary

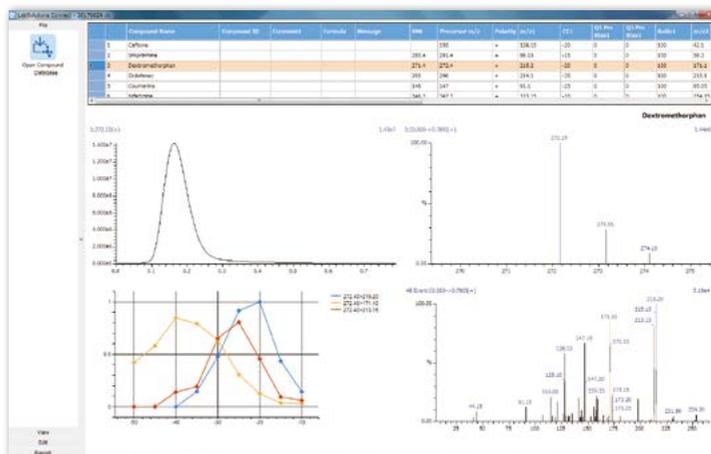
# Smart Software for Anyone Doing LC-MS/MS

## LabSolutions Connect™

LabSolutions Connect is the smart way to work for all routine laboratories. Simplifying workflows to run samples on the LC-MS/MS with tools to help MRM optimization.

### ■ Get Better Results

Laboratories with the need for expanding target compound panels or building up new methods also need to consider how to get the highest sensitivity without manual compound optimization. The automated MRM optimization tool, which is part of the LabSolutions Connect platform, delivers MRM transitions for quantitation and for MRM Spectrum for library searchable identification.



#### MRM Data Review

A simple graphical interface showing the collision energy profiles for multiple product ions

### ■ Tablet-like UI for Sample Analysis

In routine laboratories, the sample to result cycle time defines efficiency and productivity. To help reduce the sample to result cycle time and open LC-MS/MS technology to everyone the user experience has been redefined making running samples easy. LabSolutions Connect is designed with an intuitive layout to show the sample list as a simple table and the position of the sample in the autosampler tray.



#### Designed for Everyone in The Lab

By redesigning the user experience, analytical scientists across multiple disciplines can run sample lists, check the sample vials are in the right position and see the status of the instrument in one smart layout.

Its simple, intuitive and streamlines workflows in any laboratory environment.

# LabSolutions Insight™

## Rethinking Quantitative Data Review

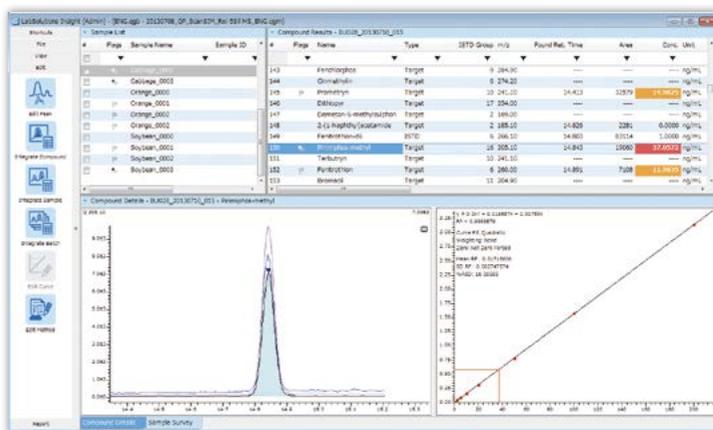
LabSolutions Insight has powerful data mining and analytics capabilities for reviewing LC-MS/MS results. It is designed to support review-by-exception enabling quality rules to identify exceptions quickly. LabSolutions Insight now has the added capability to work seamlessly with the LabSolutions DB/CS environment and audited regulatory requirements, it also has

the flexibility to adapt to different reporting workflows with multiple results files.

The new Insight software also supports library identification by either full scan or MRM spectrum mode helping to provide tools for both quantitation and identification in one workspace.

### ■ Brings A New Way to Review Actionable Data

LabSolutions Insight enables quantitative data to be reviewed in different ways, each connected workspace environment helps to check peak integration, find outliers, show chart trends and calibration curve data. Visualizing data, finding specific information, sorting actionable data is made easy by applying filters to each field in the table.



#### LabSolutions Insight

Finds actionable data faster.

LabSolutions Insight has a panel of quality rules that can be set-up to find outliers at the touch of a single click. Outliers are color coded and can be easily visualized, sorted and reported.

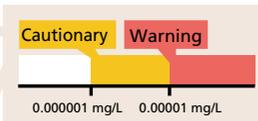
### ■ Survey Panel View to Quickly Review Actionable Data

Checking and reviewing individual data files can have a marked impact on laboratory productivity. Survey mode helps to change productivity by simply visualizing positive samples, outliers or simply to check data quality. As Insight uses dock-able pane technology, the survey mode screen can be shared on multiple monitors helping to improve productivity and data quality review for large panels of target compounds.



Sample Survey View

Color-coded flags



#### Color Coded Review

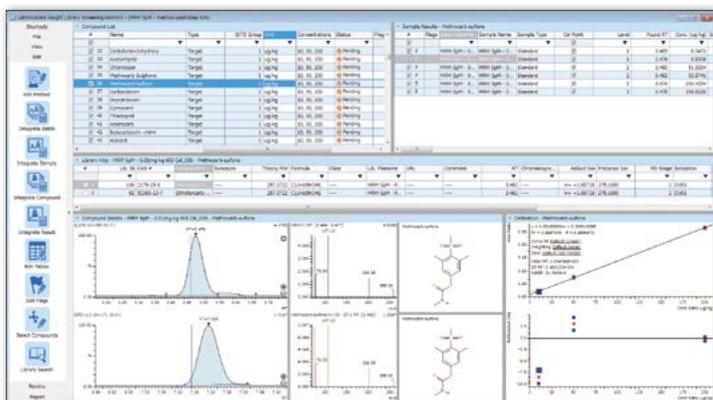
By supporting a range of quality rules, samples can be flagged if the concentration is considered cautionary or as a warning. But the possibilities can be focused to specific needs highlighting retention time variation, ion ratio tolerance outside a set range, calibration curve regression outside an expected range. The list of quality rules helps to find actionable data quickly.

# Compound Identification

## LabSolutions Insight Library Screening

LabSolutions Insight offers MS/MS library search capabilities. Instrument parameters and MS/MS library spectra are available to deliver faster data acquisition, higher data quality, and enhanced identification. Shimadzu's LabSolutions Insight software offers easy viewing of the compounds of interest, including structural information, retention time and library similarity score. LabSolutions also enables you to produce

high-quality results without the need to define a threshold value to trigger a spectrum, decreasing the chance of false negative reporting. This feature, MRM Spectrum Mode, acquires all compound fragments of interest in MRM mode and can be used to create accurate spectra from even trace concentrations.



### Example of the screening of veterinary drugs using MRM spectrum mode

In MRM Spectrum Mode, known compound fragments are selectively acquired using multiple MRM channels, enhancing signal for low abundance analytes. Shimadzu's ultra-fast quadrupole technology makes this a practical approach for large panels of analytes.

## LC/MS/MS Method Packages and MRM Libraries

A variety of method packages and MRM libraries, which include analysis conditions such as MRM parameters, enable efficient implementation of simultaneous multi-component analyses. The method parameter list included in these packages can be used to create methods that analyze targeted components only. These packages can save laboratories a great deal of method development time.



	Description	Flyer code
Method Packages	Residual Pesticides	C146-E306
	Veterinary Drugs	C146-E387
	Water Quality Analysis	C146-E180
	Rapid Toxicology Screening	C146-E224
	Primary Metabolites	C146-E227
	Lipid Mediators	C146-E381
	Cell Culture Profiling	C146-E279
	D/L Amino Acids	C146-E336
	Short Chain Fatty Acids	C146-E355
	Mycotoxins	C146-E351
	Forensic Toxicology Database	C146-E344
	Aminoglycoside Antibiotics	C146-E352
Restricted Chemicals in Textiles	C146-E382	
MRM Libraries	Metabolic Enzymes in Yeast	C146-E275
	Phospholipid Profiling	C146-E314

Note: Optimization of analysis parameters will be necessary in some cases when using the LCMS-8045.

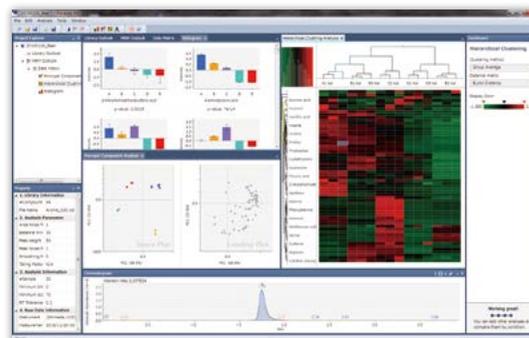
## Traverse MS™

Multivariate Analysis Software Supports MRM Data

Traverse MS data analysis software is intended for high-speed processing of MRM data acquired with Shimadzu triple quadrupole LCMS systems in the field of targeted metabolomics.

Using multiple samples and multiple components, the software is able to create graphical and statistical analysis for metabolic pathway analysis.

(Brochure: C146-E308)



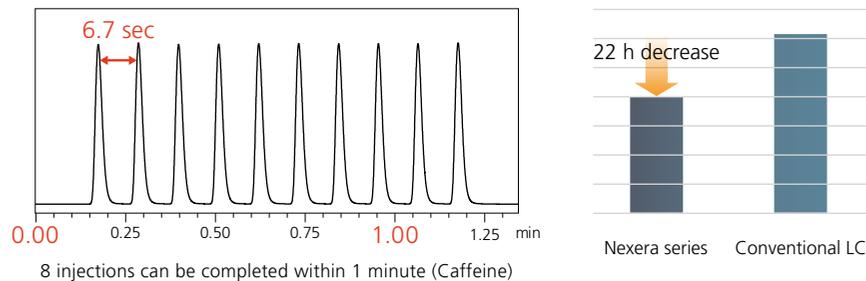
# Shimadzu Nexera™ Series

Shimadzu's unique approach to delivering high-quality, high-speed LC-MS/MS analysis combines the Shimadzu UHPLC and LCMS-8045 as a seamlessly integrated system.

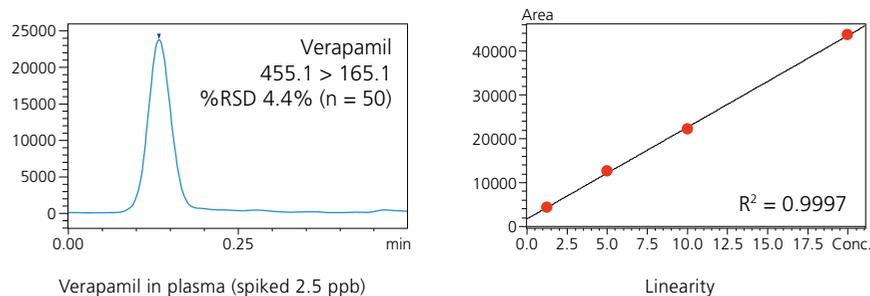


## ■ Analysis Cycle Time Less Than 10 Seconds

The SIL-40 autosampler can process the entire injection cycle time in as little as seven seconds, twice as fast as the previous model. In addition, continuous analysis can be carried out on up to 44 MTPs (using 3 PLATE CHANGERS). Together these features dramatically increase analysis throughput.

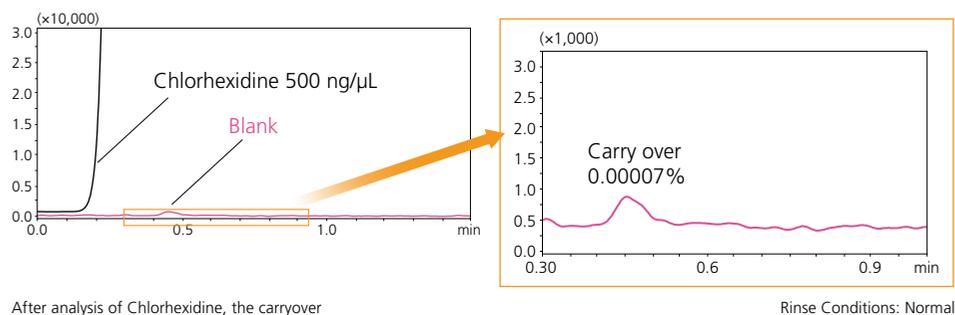


Pharmacokinetic analysis requires not only speed but also high reliability at low concentrations. With its ultra-fast injection and ultra-low carryover, the SIL-40 autosampler delivers high reproducibility and reliability, even during an ultra-fast 30-second analysis.



## ■ Ultra-low Carryover

The Nexera boasts ultra-low carryover, even on a high-sensitivity LC-MS/MS. This reduces time spent on rinsing, resulting in a shorter overall analysis time.



After analysis of Chlorhexidine, the carryover to a blank solution is negligible.

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