

Liquid Chromatograph Mass Spectrometer

LCMS-8040

UFMS
ULTRA FAST MASS SPECTROMETRY



LCMS-8040

SHIMADZU

LIQUID CHROMATOGRAPH MASS SPECTROMETER

W
GAS
HEATER
STATUS
POWER

LCMS-8040

— *Enhanced Sensitivity*



■ Ultra-High Sensitivity

By incorporating newly improved ion optics and collision cell technology, the LCMS-8040 provides higher multiple reaction monitoring (MRM) sensitivity. A five-fold increase in sensitivity (reserpine, S/N ratio), as compared with that of LCMS-8030 has been achieved by improving ion focusing and minimizing ion losses between multi-pole lenses. These improvements also yield higher sensitivity for scan mode measurements. This higher sensitivity expands the potential range of LC/MS/MS applications.

■ Ultra-High Speed

The LCMS-8040 was designed to provide significantly higher sensitivity while maintaining the high speed offered by the LCMS-8030. Ultrafast MRM transition speeds, up to 555 MRMs per second, are achieved by Shimadzu's UFsweeper collision cell technology, proprietary high-precision quadrupole machining capabilities, and unique high voltage power supply technology. In addition, the LCMS-8040 features the fast polarity switching at 15 msec. With this high-speed performance, the LCMS-8040 can dramatically improve analytical throughput.

■ Ultra-High Reliability

MRM optimization in Shimadzu's LCMS systems is based on a rapid series of automated flow injection analyses, requiring only minutes to perform. Multiple compounds can be optimized in an unattended sequence, freeing the analyst from tedious work. MRM parameters optimized for the LCMS-8030 can be transferred to the LCMS-8040, making it possible to transfer methods between systems. The LCMS-8040 offers the same ease of maintenance benefits as the LCMS-8030, and all consumables, such as desolvation lines (DL) and ESI capillaries, are interchangeable as well.

UFMS
ULTRA FAST MASS SPECTROMETRY

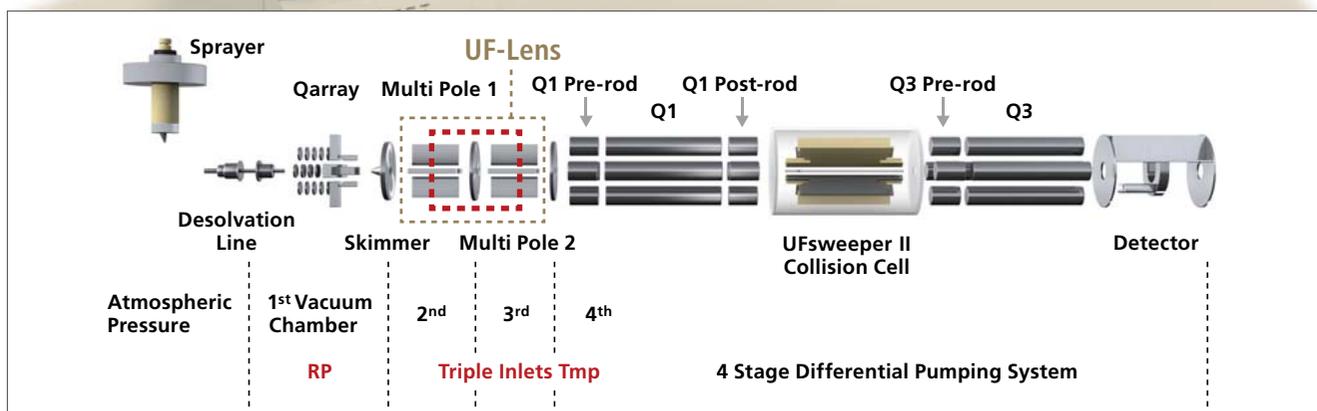
Speed Beyond Comparison

Ultra-High Sensitivity with UFMS Technology

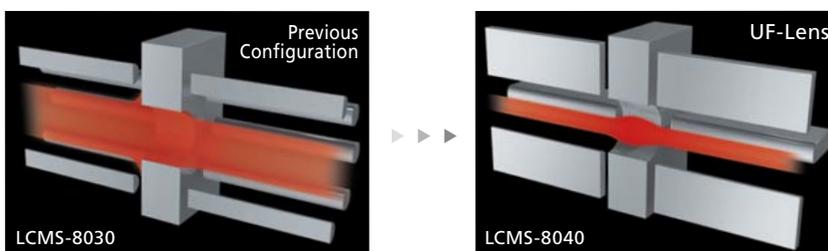
Higher Sensitivity with Improved Ion Optics

UF-Lens

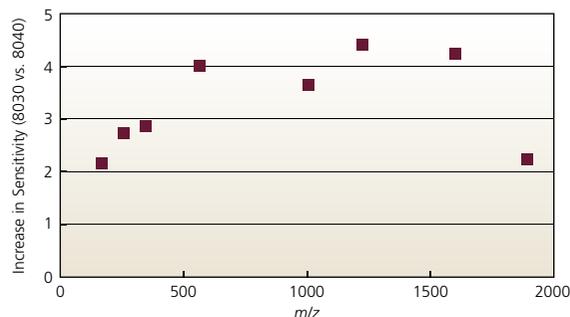
The UF-Lens is a lens system that offers both higher sensitivity and easier maintenance. The optical system integrates two multi-pole RF ion guides for higher sensitivity. In addition, the lens system can be removed without tools for easy cleaning.



Ion losses between segments are minimized by utilizing quadrupole ion guides.



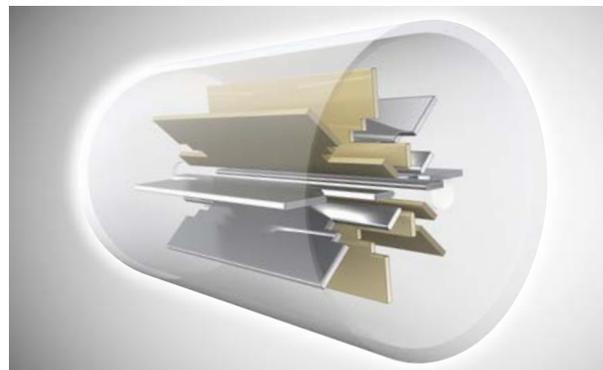
A comparison of auto-tune Q1 scan results for a standard sample (a mixture of PEG, PPG, and raffinose) obtained from the LCMS-8030 and LCMS-8040 is shown to the right. Target ions used for ESI+ auto-tuning are plotted (m/z 65.05, 168.10, 256.15, 344.20, 652.40, 1004.60, and 1224.75). A significant sensitivity increase across a broad molecular weight range for precursor ion transmission is demonstrated.



Higher CID Efficiency with Improved Collision Cell

UFsweeper II

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.

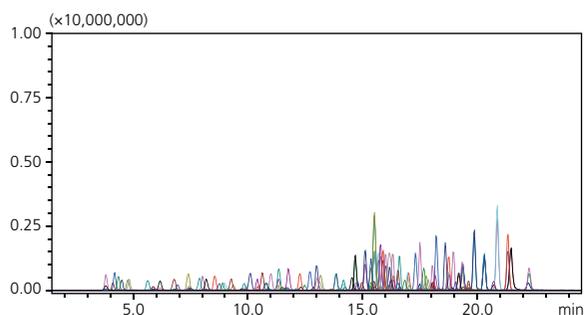


Sample Name	Precursor <i>m/z</i>	Product <i>m/z</i>	LCMS-8030 CID efficiency	LCMS-8040 CID efficiency	Proportional Increase
Lidocaine	235.4	86.1	20.0	29.0	1.4
Atropine	290.1	124.1	7.2	11.0	1.5
Yohimbine	355.1	144.0	9.5	15.6	1.6
Tetracaine	265.1	176.1	15.7	32.0	2.0
Doxepin	280.1	107.1	4.4	7.2	1.6
Imipramine	281.1	86.1	16.2	22.1	1.3
Nortriptyline	264.1	233.1	3.8	7.4	1.9
Isopropylantipyrine	231.1	188.9	1.5	2.9	1.9
Diazepam	285.0	154.0	2.4	3.9	1.6
Reserpine	609.3	195.1	3.9	6.6	1.7

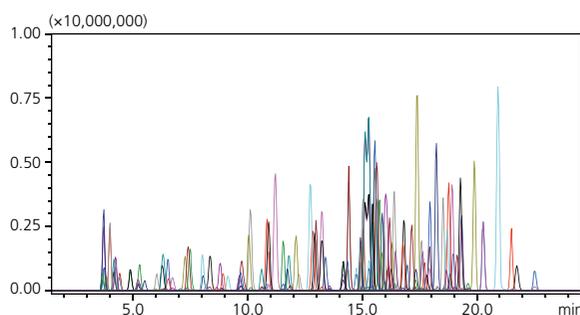
The LCMS-8040 offers higher sensitivity while maintaining the ultrafast performance of the LCMS-8030. The figures below show simultaneous analysis of 167 pesticides in MRM positive/negative ion analysis mode. Even though positive and negative ions were

measured simultaneously, both the LCMS-8030 and LCMS-8040 accurately identified all 167 components. In addition, the LCMS-8040 showed improved sensitivity – an average of three times higher for all components.

■ LCMS-8030



■ LCMS-8040



HPLC

Analysis Column	Shim-pack FC-ODS (2.0 mm I.D. x 150 mm L., 3 μm)
Mobile Phase A	5 mmol/L ammonium acetate - Water
Mobile Phase B	5 mmol/L ammonium acetate - Methanol
Gradient Program	15%B (0 min) – 40%B (1–3.5 min) – 50%B (6 min) – 55%B (8 min) – 95%B (17.5–30 min) – 15%B (30.01–40 min)
Flow Rate	0.2 mL/min
Column Temperature	40°C

MS

Probe Voltage	+4.5 kV (ESI-Positive mode) / -3.5 kV (ESI-Negative mode)
Nebulizing Gas Flow	1.5 L/min
Drying Gas Flow	10 L/min
DL Temperature	250°C
Heat Block Temperature	400°C

Proven Ultra-High Performance now with Enhanced Sensitivity

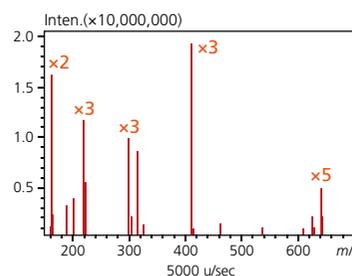
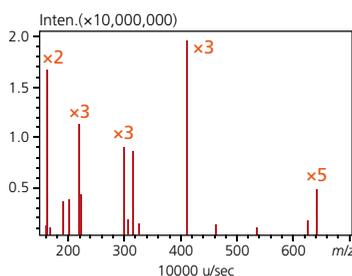
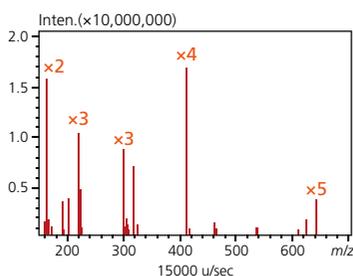
Higher Sensitivity for Q1 Full Scan Spectra

The LCMS-8040 maintains the same high-speed scanning (UFscanning) and polarity switching technology (UFswitching) utilized in the LCMS-8030.

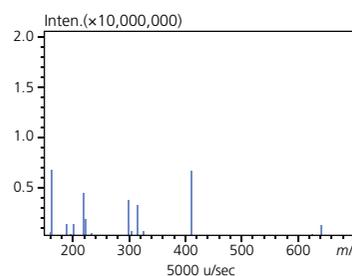
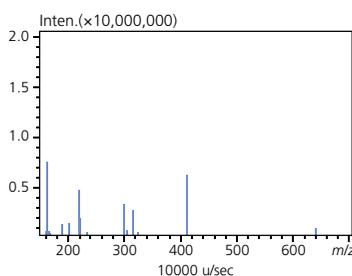
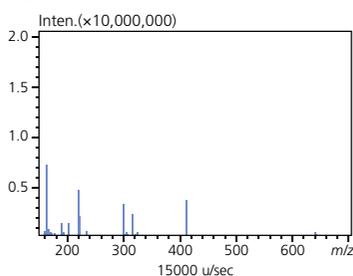
The LCMS-8040 not only maintains Shimadzu's proprietary high-speed technologies (UF Technologies, USP7855355, USP8188426), which minimize sensitivity losses even at faster scan speeds, it also features improved ion optics, which provide higher sensitivity for MRMs and full scans. A comparison of Q1 full scan spectra for

pesticide samples (Methomyl, Carbaryl(NAC), Phoxim, Benfuracarb, and Abamectin B1a) is shown below. The upper spectra were acquired using the LCMS-8040 and the lower spectra were acquired using the LCMS-8030. As shown, the LCMS-8040 offers significant sensitivity improvements for precursor ions or full scan data.

LCMS-8040



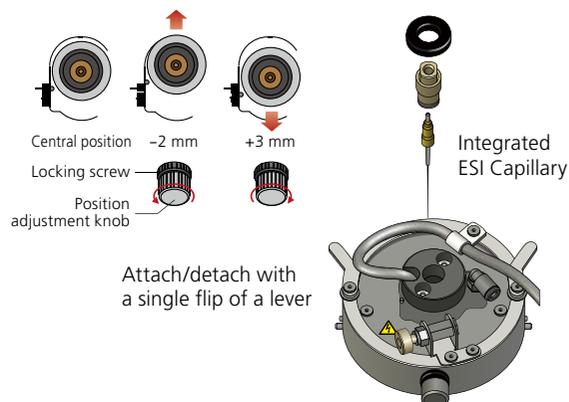
LCMS-8030



Proven Interface for Robust Performance

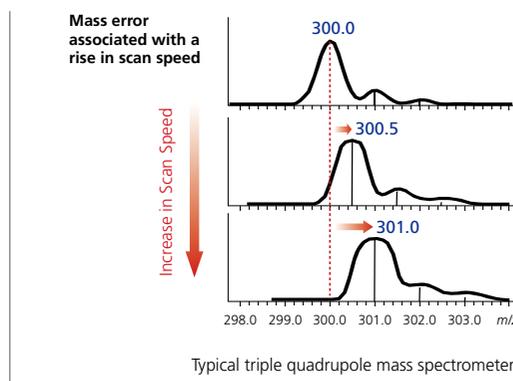
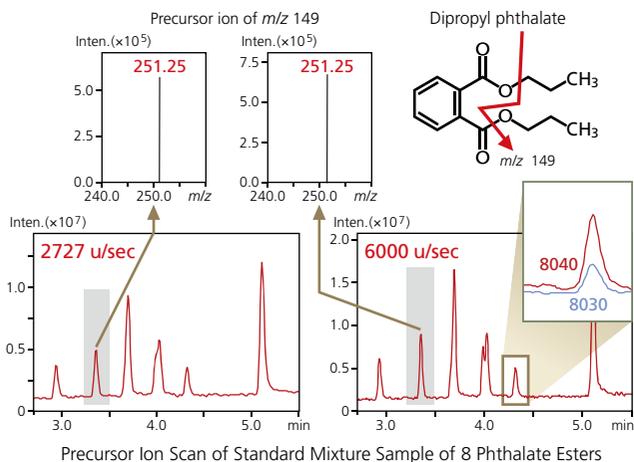
Robust, User-Friendly Interface

The LCMS-8030 and LCMS-8040 use the same interface. In LCMS analysis, it is necessary to adjust interface conditions such as temperatures and gas flow rates for optimal desolvation. Spray needle adjustment and probe position are also factors to be evaluated. In both the LCMS-8030 and LCMS-8040, temperatures and flows are easily controlled through the software. ESI probe position is set by a single easily accessible knob, and spray needle protrusion is adjusted without the need for any special tools or disassembly of the probe. In addition, this capillary incorporates a tapered design, which reduces sample clogging.



Higher Sensitivity for MS/MS Acquisition Modes

The increased scan sensitivity of the LCMS-8040 also applies to scan modes specific to triple quadrupole mass spectrometers, such as product ion scanning, precursor ion scanning, and neutral loss scanning. Historically, mass spectrometers have introduced mass deviation in linked scans, such as precursor ion scans or neutral loss scans, when measured at maximum scan speeds.



However, Shimadzu's proprietary UFscanning technology allows performing precursor ion scans or neutral loss scans at high speeds without loss of mass accuracy. In addition, the LCMS-8040 offers higher sensitivity levels. Precursor scan results for eight kinds of phthalate esters are shown to the left. Scans were performed at two speeds, 2727 u/sec and 6000 u/sec. No mass shift is observed at either scan speed, and a significant sensitivity improvement is observed for the LCMS-8040.

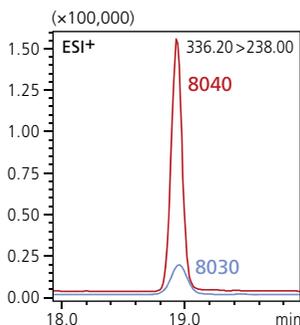
Easy Method Transfer

MRM parameters for the LCMS-8030 can be used in LCMS-8040 systems.

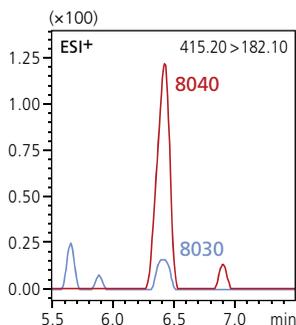
Optimization of MRM parameters is an early step in LCMS method development. Shimadzu has streamlined the MRM optimization process with a rapid and simplified approach based on automated flow injection analysis. Several method packages, which contain chromatographic and optimized MRM conditions for a variety of analytes, including residual pesticides, veterinary drugs, and forensic drugs of abuse, have also been released. Laboratories

employing LCMS-8030 MRM conditions will be able to transfer these MRMs directly to the LCMS-8040. To demonstrate this, a method for the simultaneous analysis of 167 pesticides was transferred without modification from the LCMS-8030 to the LCMS-8040. Increased sensitivity was obtained for all compounds; three example chromatograms are shown below.

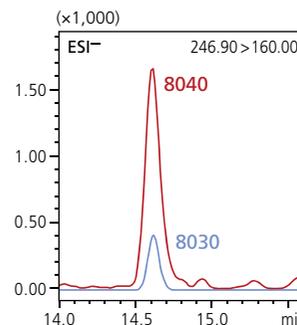
10 ppb: Cloquintocet-mexyl (9.5X)



10 ppb: Pyrazosulfuron-ethyl (7.4X)



10 ppb: Linuron (5.2X)

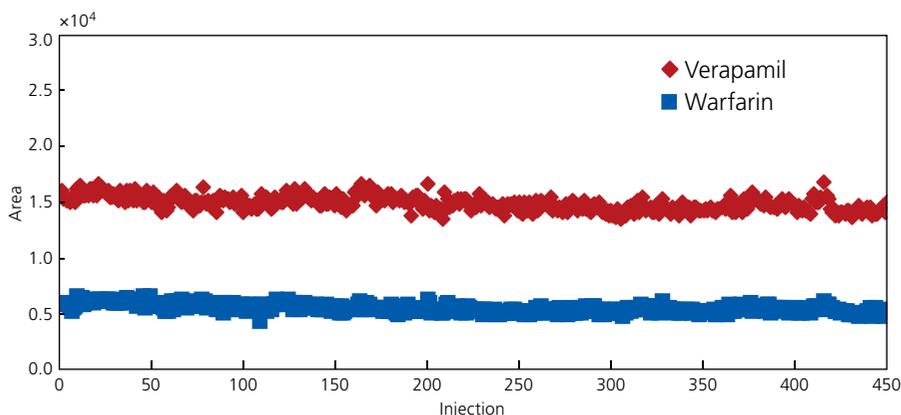


Ultra-High Reliability to Withstand Wide Range of Complex Matrices

Exceptional Durability

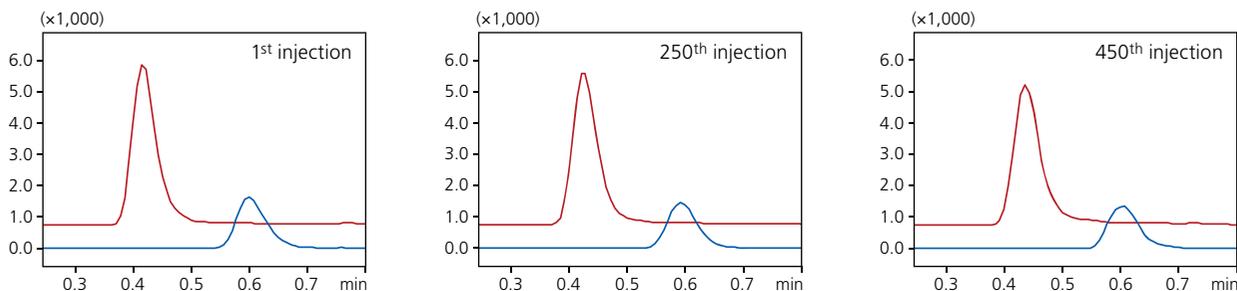
Blood plasma samples were spiked with verapamil and warfarin, and then deproteinized according to the pretreatment process indicated below. The area values from 450 consecutive LCMS-8040 analyses were then plotted. Simultaneous analysis of verapamil by ESI+ and

warfarin by ESI- was performed. Chromatograms for the 1st, 250th, and 450th measurements are shown below. This resulted in 1 pg on-column area repeatability of 4.18% for verapamil and 6.61% for warfarin.



Column: Shim-pack XR-ODS II (2.0 mm I.D. × 50 mm L, 2.2 μm)
 Mobile Phase A: 5 mmol/L ammonium acetate–water
 Mobile Phase B: Acetonitrile
 Gradient Program:
 60% B (0–1.50 min) –
 90% B (1.51–3.00 min) –
 60% B (3.01–4.50 min)
 Flow Rate: 0.4 mL/min.

200 μL plasma sample
 Add 200 μL Acetonitrile, 50 μL 50% methanol aqueous solution and 50 μL verapamil and warfarin standard solutions.
 Vortex and centrifuge (10000 rpm, 3 min.) followed by freeze drying.
 Add 500 μL dilution solution.
 Vortex and centrifuge (12000 rpm, 5 min.).

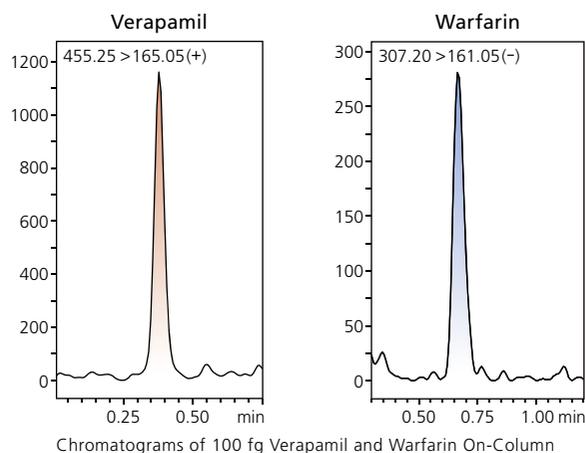


Ultra Fast Speed Combined with Lower Femtogram Detection

Using the same chromatography parameters as described above, analysis of plasma samples spiked with 40 fg/μL verapamil and warfarin were injected into the LCMS-8040 for signal to noise determination. For 100 fg on-column, a S/N ratio of 146 (rms) was obtained for verapamil and 30 (rms) for warfarin.

The resulting lower limits of detection for S/N = 3 (rms) were 2.05 fg for verapamil and 9.88 fg for warfarin.

Compounds	Verapamil	Warfarin
S/N: 100 fg on column (rms)	146	30
LOD (fg) Calculated at S/N = 3	2.05	9.88

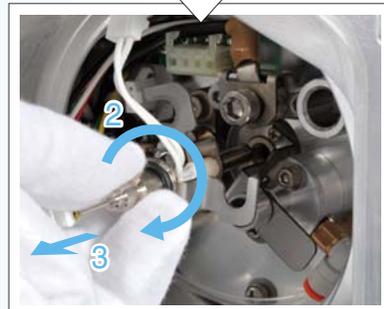


Chromatograms of 100 fg Verapamil and Warfarin On-Column

Optimizing System Performance

The LCMS-8030 heated ion source works with the most challenging samples, delivering robust, high-sensitivity detection using ESI, APCI or our dual probe ionization interface.

System maintenance for the ion source is simplicity itself. Cleaning the heated desolvation capillary is quick and maintains system vacuum to provide greater uptime and usability.



Easy Maintenance Identical to the LCMS-2020

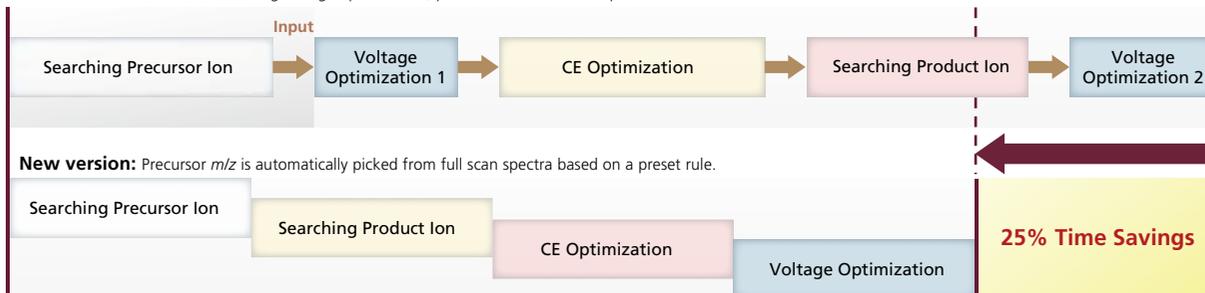
LabSolutions LCMS

Shimadzu's data acquisition software provides a single point of control for LC and MS parameters. In addition, by incorporating critical input from customers, Shimadzu provides laboratories with software tools to address specific laboratory workflows and improve productivity.

Fully Automated MRM Optimization

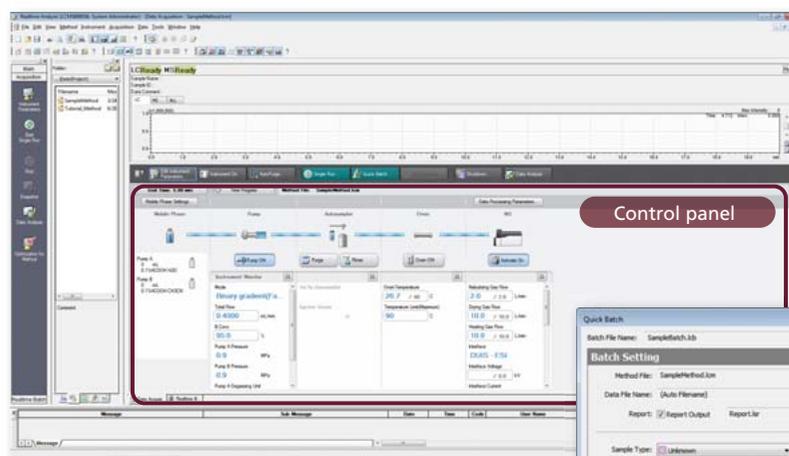
It's faster and easier to optimize quantitative parameters with updated software that reduces MRM optimization time by 25%.

Previous version: Before starting voltage optimization, precursor m/z must be input.



Intuitive User Interface

A new approach helps simplify the user experience for high-throughput laboratories. Quick batch makes it easier to perform routine LC/MS/MS analyses and changes to the Control Panel help method development.

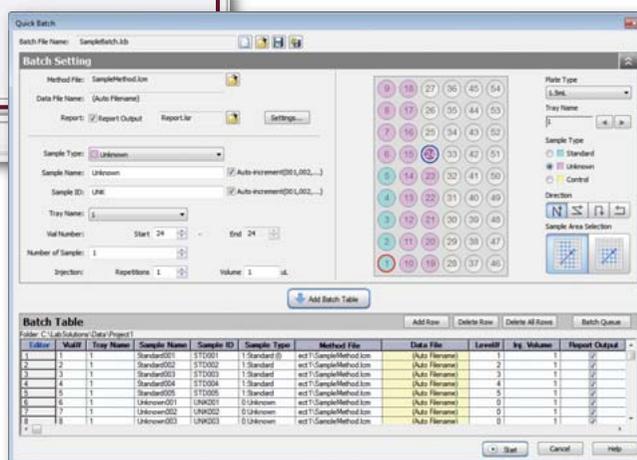


Method development

An updated Control Panel makes it easier to change LC/MS/MS methods.

Quick Batch

Streamlines sample submission. A simple color-coded autosampler graphic offers quick visualization of the sample queue. Three color codes have been designed for standards (sky blue), unknowns (purple) and controls (yellow).



Automatic Calculation of Dwell Time

The optimum dwell time is calculated automatically from the number of overlapping MRM channels and maximum loop time, thereby obtaining the necessary data points for the entire analysis.

Type	Event#	n/f	Compound Name	m/z	Time (2.000 min - 7.500 min)
MRM	5	+	HT 2 442 10-262 95		
MRM	6	+	FMB1 722 26-334 20		
MRM	7	+	FMB2 83 706 26-336 30		
MRM	8	+	T 2 484 65-185 00		
MRM	9	+	OFA 403 90-238 90		
MRM	10	-	PAT 153 00-109 00		
MRM	11	-	NPV 370 50-280 45		
MRM	12	-	QON 354 90-298 95		
MRM	13	-	ZON 317 15-273 10		
MRM	14	-	ZON 317 20-131 20		

Start - End Time(min)	2.000-	4.000-	4.500-	5.000-	6.000-	6.500-	7.0
Event	3	8	9	11	7	3	
Loop Time(sec)	0.903	1.298	1.099	1.201	1.017	0.363	
Dwell Time(msec)	150.0-500.0	30.0-500.0	30.0-250.0	30.0-200.0	50.0-200.0	50.0-150.0	

Maximum Event: 11 Maximum Loop Time(sec): 1.298
 Minimum Dwell Time(msec): 30.0
 Maximum Dwell Time(msec): 500.0

Optional Software Programs

Shimadzu offers numerous options to address specific customer requirements. Combining LabSolutions LCMS with these programs improves workflow efficiency.

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.



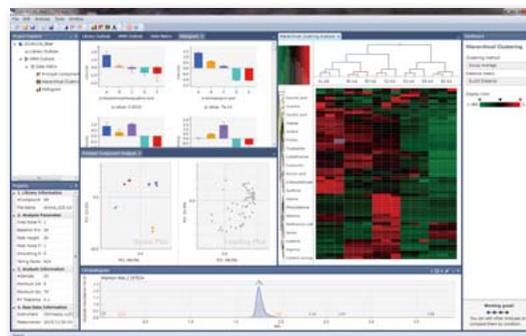
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Method Packages	Residual Pesticides	C146-E306
	Veterinary Drugs	C146-E161
	Water Quality Analysis	C146-E180
	Drugs of Abuse	C146-E181
	Rapid Toxicology Screening	C146-E224
	Primary Metabolites	C146-E227
	Lipid Mediators	C146-E225
	Cell Culture Profiling	C146-E279
MRM Libraries	Metabolic Enzymes in Yeast	C146-E275
	Phospholipid Profiling	C146-E314

*Optimization of analysis parameters will be necessary in some cases when using the LCMS-8040.

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 Corporation

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