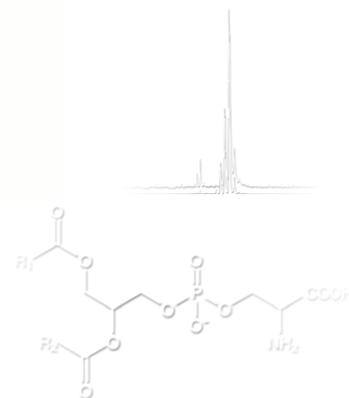


Shimadzu's Mass Spectrometry Solutions

# Mass Spectrometry General Product Catalog

**UFMS**  
ULTRA FAST MASS SPECTROMETRY



# Providing Excellence in Data Quality and Ultra-Fast Performance, Shimadzu's Unique Technologies Achieve a New Global Standard in Mass Spectrometry

## *Speed Beyond Comparison* **UFMS** *ULTRA FAST MASS SPECTROMETRY*

Shimadzu Corporation, a leader in the development of advanced technologies, introduces two new triple quadrupole mass spectrometers: LCMS-8060 and GCMS-TQ8040. The LCMS-8060 provides the highest sensitivity for the analytical market while the GCMS-TQ8040 establishes a new benchmark in Shimadzu's history of GC-MS innovation.

These new additions to the Ultra-Fast Mass Spectrometry (UFMS) series are characterized by Shimadzu's proprietary ultra-fast technologies.

The UFMS series provides high-sensitivity performance and greater excellence in data quality, enabling dramatic improvements in laboratory throughput for an ever-widening range of analytical applications.

Utilizing the same user-friendly interface as HPLC/UHPLC and GC modules, LabSolutions MS workstation software provides intuitive functionality for more efficient data processing and an easier, more productive analytical workflow.

### Shimadzu's UFMS Series



iMScope *TRIO*\*



LCMS-8060



GCMS-TQ8040



MALDI-7090



LCMS-8050



LCMS-8040



LCMS-8030



LCMS-2020



LCMS-IT-TOF



GCMS-QP2010 Ultra  
GCMS-QP2010 SE

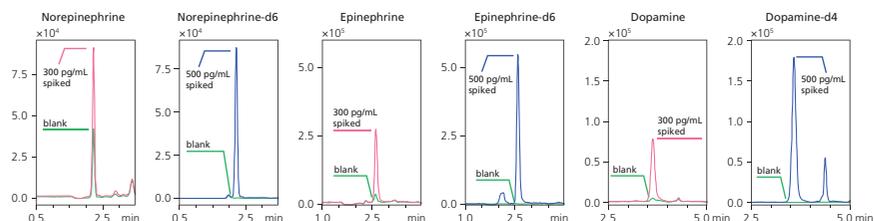
\* iMScope *TRIO* may not be sold in your country. Please contact us to check the availability of this product in your country.

# Mass Spectrometer Lineup

High-Throughput Liquid Chromatograph Mass Spectrometer

## LCMS-8060

The newest model in the Ultra-Fast Mass Spectrometry series, the LCMS-8060 delivers the highest sensitivity and fastest analysis speed of any LCMS on the market today. In conjunction with a robust design and easy maintenance, the LCMS-8060 offers the ideal solution for better data quality and higher throughput for a wide array of challenging and routine applications.

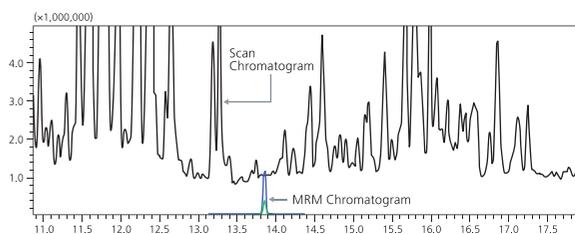


Detection of Norepinephrine, Epinephrine and Dopamine and their deuterated internal standards in plasma

Ultra-Fast Gas Chromatograph Mass Spectrometer

## GCMS-TQ8040

The GCMS-TQ8040 triple quadrupole GC-MS/MS features the fastest scan speed in the industry, making it the only GC-MS/MS capable of running simultaneous TQ modes and scan mode, e.g. Scan/MRM or Scan/SIM/MRM. Combined with high-sensitivity ion optics, the GCMS-TQ8040 provides a state-of-the-art solution for all of today's applications, from food safety to environmental monitoring, clinical research, and forensics.

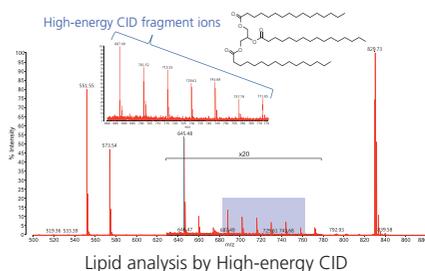


Analysis of Pesticides in a Cabbage Extract Using Scan/MRM

MALDI TOF-TOF Mass Spectrometer

## MALDI-7090

The MALDI-7090™ is a high performance MALDI TOF-TOF mass spectrometer combining high-throughput, high resolution and high-energy CID and has been designed primarily to address the proteomics and tissue imaging markets. The combination of Shimadzu's extensive MALDI-TOF-TOF expertise with novel patented technology provides the MALDI-7090 with ultimate capabilities for identification and structural characterization of biomolecules.



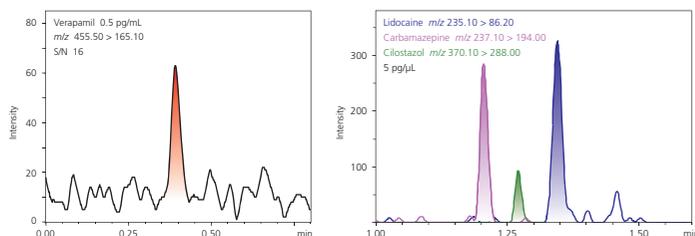
# Mass Spectrometer Lineup



High-Throughput Liquid Chromatograph Mass Spectrometer

## LCMS-8050

The LCMS-8050 triple quadrupole LC-MS/MS system provides both best-in-class sensitivity and excellent quantitation performance. This excellent sensitivity is maintained even in the most difficult matrices, making the LCMS-8050 excellent for drug discovery, manufacturing, clinical research, food safety, environmental, or drugs of abuse analysis. Integrated control and analysis software enables an efficient, user-friendly workflow.



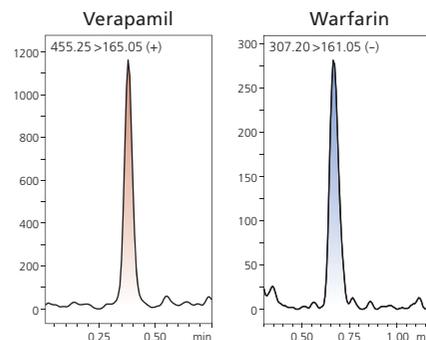
MRM chromatogram of verapamil (0.5 pg/mL) and lidocaine, carbamazepine and clobazepam (5 pg/mL)



High-Throughput Liquid Chromatograph Mass Spectrometer

## LCMS-8040

The LCMS-8040 is an ultra-fast triple quadrupole LC-MS/MS providing enhanced sensitivity for complex matrices and difficult analytes. It retains the rapid MRM and polarity switching capabilities of the LCMS-8030, while incorporating improved ion optics for increased sensitivity.



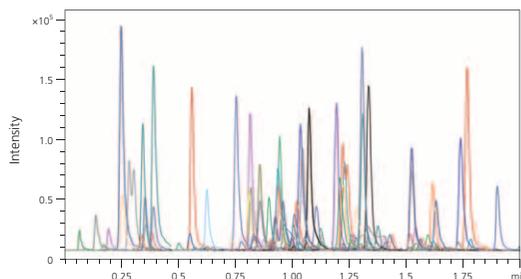
Chromatograms of 100 fg Verapamil and Warfarin On-Column



High-Throughput Liquid Chromatograph Mass Spectrometer

## LCMS-8030

The LCMS-8030 is a next-generation ultra-fast LC-MS/MS detector for use with UHPLC or standard HPLC systems. Ultra-fast positive-negative polarity switching and ultra-fast scan speeds maximize analytical throughput.



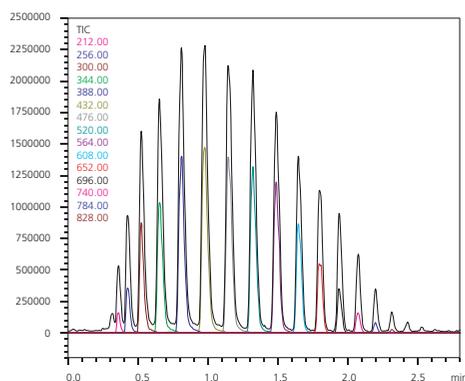
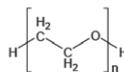
Simultaneous MRM Positive-Negative chromatogram of 226 Pesticide Components (10 ng/mL)

High-Throughput Liquid Chromatograph Mass Spectrometer

## LCMS-2020

The LCMS-2020 is an ultra-fast liquid chromatograph mass spectrometer designed for ease of use as an HPLC or UHPLC detector.

This single quadrupole detector offers faster measurements and higher detection sensitivity for quicker and more accurate detection of trace impurities in a variety of applications.



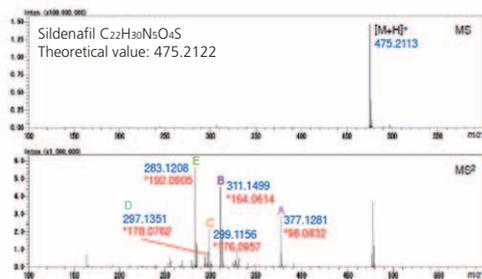
Mass Chromatogram of Polyethylene Glycol 400



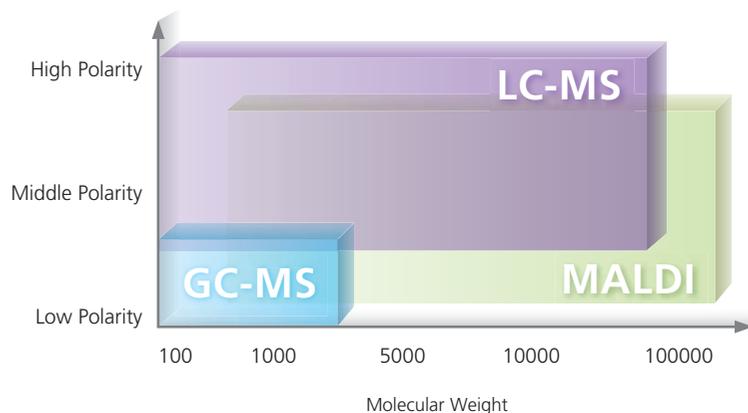
High-Throughput Liquid Chromatograph Mass Spectrometer

## LCMS-IT-TOF

The LCMS-IT-TOF system is a hybrid high performance liquid chromatograph ion trap (IT) and time-of-flight (TOF) mass spectrometer. The IT provides MS<sup>n</sup> capability, which is coupled with the high resolution and high mass accuracy capability of TOF.



Mass Spectra of Sildenafil



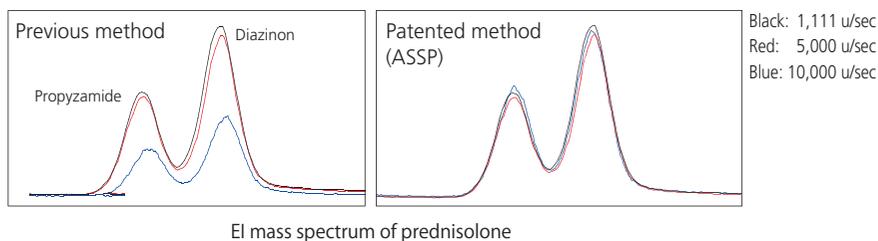
# Mass Spectrometer Lineup



Sensitive, High-Speed Gas Chromatograph Mass Spectrometer

## GCMS-QP2010 *Ultra* SE

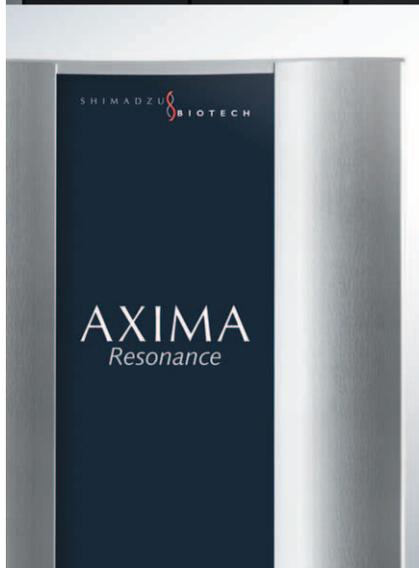
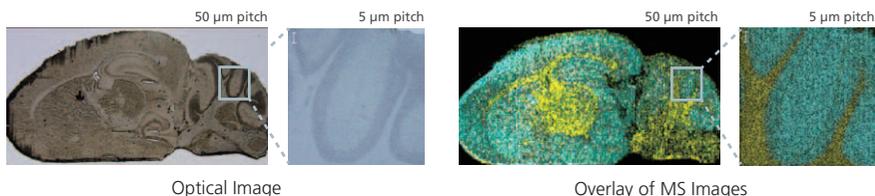
The GCMS-QP2010 Ultra utilizes patented Advanced Scanning Speed Protocol (ASSP®) technology, allowing high-speed scanning at 20,000 u/second without sensitivity loss or spectral distortion. A versatile, robust solution, the GCMS-QP2010 SE offers reliable, cost-effective productivity for the most challenging laboratory analyses.



Imaging Mass Microscope

## iMScope *TRIO*

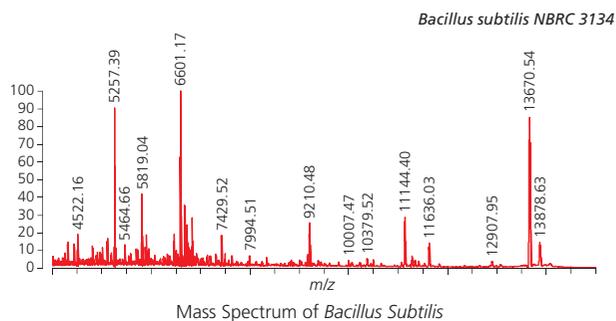
Imaging mass spectrometry is a revolutionary new technology. This instrument is a combination of an optical microscope, which allows the observation of high-resolution morphological images, with a mass spectrometer, which identifies and visualizes the distribution of specific molecules. Superimposing the two images obtained based on these very different principles creates a significant new research tool. The accurate and high resolution mass images from the iMScope TRIO will drive your research to the next level.



Matrix Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometer

## AXIMA Series

The AXIMA series includes four MALDI-TOF MS models, ranging from a linear-only model to hybrid ion trap TOF. A key feature of MALDI-TOF MS systems is their ability to acquire mass spectra directly from crude samples, such as tissue specimens and microorganisms.



# Mass spectrometers must first ionize sample molecules.

Many types of ionization have been developed.

Electron ionization (EI) ionizes molecules using accelerated thermal electrons, 70 eV. EI is generally used for molecules whose molecular weight is less than 1000. It is typically used in combination with a gas chromatograph to analyze highly volatile or gaseous molecules.

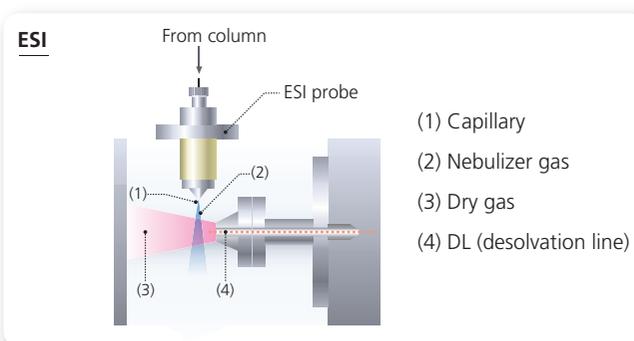
Electrospray ionization (ESI) requires a liquid stream to be dispersed into an aerosol. It is mainly used in combination with liquid chromatographs.

Matrix Assisted Laser Desorption/Ionization (MALDI) desorbs sample molecules with laser energy and ionizes them via charge transfer from matrix ions. MALDI can be applied to a wide range of samples by changing matrix reagents; hence, this ionization method applies to synthetic polymers and other complex samples.

## ESI (Electrospray Ionization)

A sample solution is introduced to a capillary and a high voltage is applied. Nebulization gas is introduced, and charged droplets result. The droplets are reduced in size through desolvation, and gas phase ions enter the mass spectrometer.

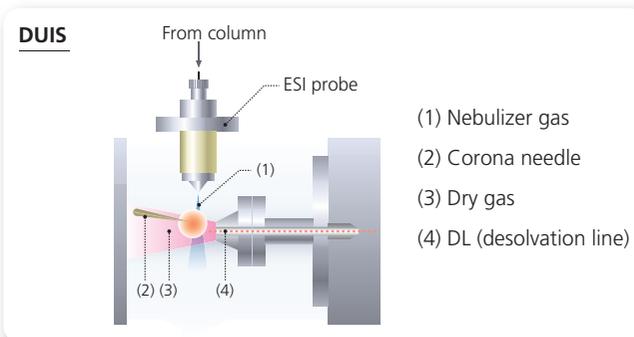
ESI is best suited to ionizing medium-to-high polarity substances, peptides, proteins, and oligonucleotides.



## DUIS (ESI+APCI)

Shimadzu's DUIS is a dual ion source that ionizes samples using both ESI and APCI (atmospheric pressure chemical ionization) modes.

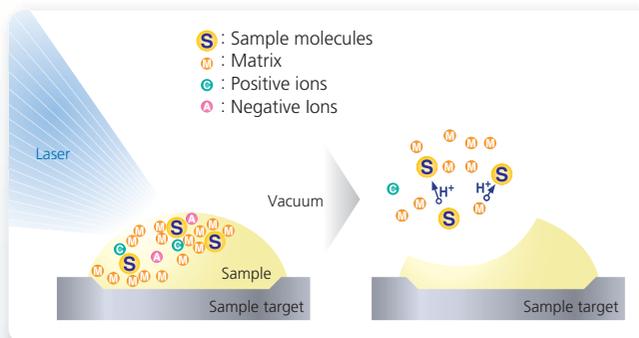
This allows both moderate and high-polarity molecules to be analyzed simultaneously.



## MALDI (Matrix Assisted Laser Desorption/Ionization)

After applying the sample and matrix solution on a sample target and drying, a laser irradiates the sample spot. The sample and matrix molecules are desorbed and ionized rapidly.

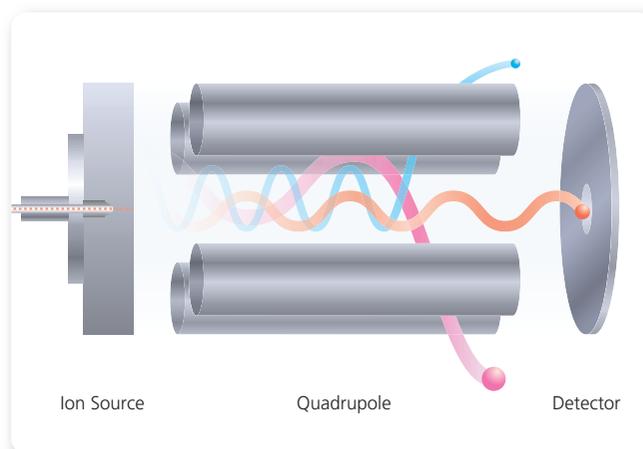
MALDI enables the ionization of high molecular weight compounds, such as proteins and polymers, without dissociation.



Sample ions are separated and detected based on differences in their mass-to-charge ratio ( $m/z$  value).

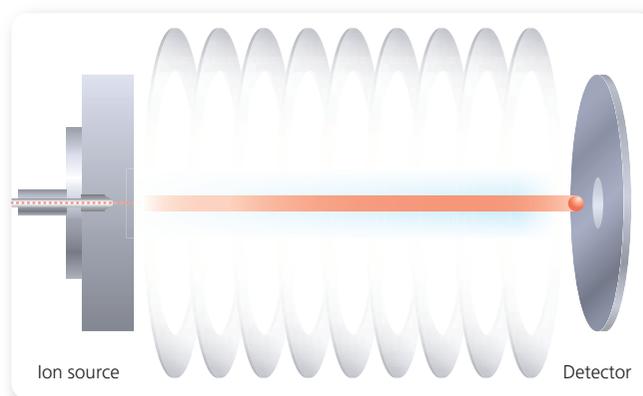
## Quadrupole Models

Quadrupole mass spectrometers use a set of four parallel electrode rods to form an electric field. The electric field is oscillated and ions passing through the field are separated by their  $m/z$  value. Triple quadrupole mass spectrometers use three sets of quadrupoles configured in series to quantitatively analyze target molecules in highly complex matrices, such as pesticides in foods, with extremely high sensitivity.



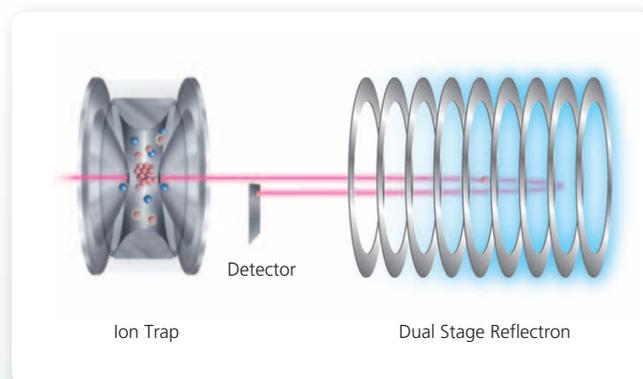
## Time-of-Flight (TOF) Models

The velocity of ions accelerated by a fixed electric voltage depends on the ions'  $m/z$  value, with smaller  $m/z$  ions moving faster. The ion flight time over a fixed distance is measured and high mass accuracy results are obtained.



## Hybrid Models

Hybrid mass spectrometers combine different types of mass spectrometers. An ion trap uses a combination of electrodes to retain ions in an electric field. Trapped ions can be subjected to a series of fragmentations, resulting in high-sensitivity  $MS^n$  analysis. In combination with time-of-flight, accurate mass information for each of these  $MS^n$  experiments can be obtained.



# The Analysis Mode of a Triple Quadrupole Mass Spectrometer

The major constituent parts of triple quadrupole mass spectrometer, starting from the ionization probe, are Quadrupole 1 (Q1), Quadrupole 2 (Q2), and Quadrupole 3 (Q3).

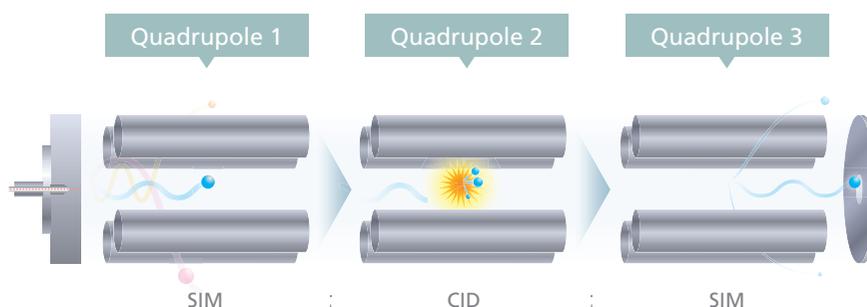
Q1 selects the precursor ions, Q2 at the center is the collision cell that smashes the ions, and Q3 selects the product ions. As the two quadrupoles Q1 and Q3 are connected in series, they are also called tandem quadrupoles.

Triple Quadrupole Mass Spectrometers are used for some quantitative analyses by changing the ion selection mode of Q1 and Q3.

## MRM (SRM)

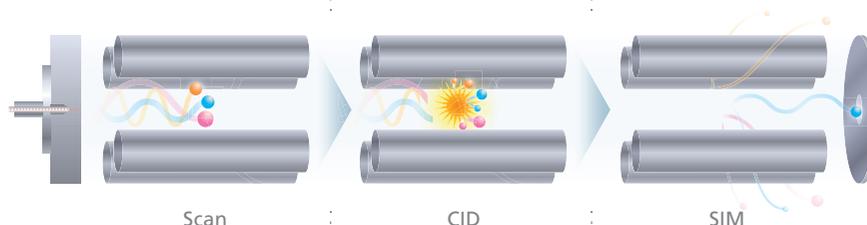
Both Q1 and Q3 are fixed at specific  $m/z$  values to selectively analyze the ions. Q1 selects specific precursor ions. Q3 selects the product ion created by collisions with an inert gas in the collision cell Q2.

MRM permits highly selective quantitative analysis, as designated precursor ions and product ions are monitored.



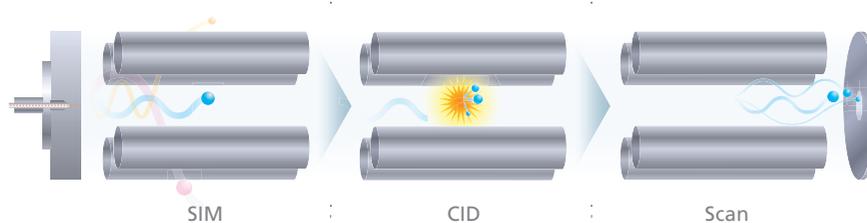
## Precursor Ion Scan

Q1 passes the ions in a certain  $m/z$  range. Q3 selects the product ion created by collisions in the collision cell Q2. Precursor ion scan permits quantitative analysis of a total amount of the molecules, including specific easily ionized functional groups.



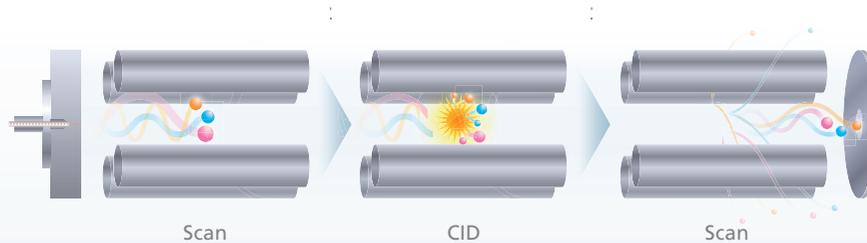
## Product Ion Scan

Q1 is fixed at a specific  $m/z$  value to select specific precursor ions. Q3 passes all product ions created in the collision cell Q2. Product ion scan permits the identification of interesting molecules.



## Neutral Loss Scan

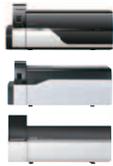
Q1 and Q3 scan in a certain  $m/z$  range while keeping a specific  $m/z$  difference. Q3 selects the product ion, which loss a specific residual group from a product ion. Neutral loss scan permits quantitative analysis of a total amount of molecules, including easily neutral loss functional groups, i.e. the hydroxyl group and phosphate group.



# Application Guide

Mass spectrometers are high-sensitivity instruments capable of obtaining both molecular weight and structural information. Consequently, they can be used for both quantitative and qualitative analyses. However, because of the wide variety of available MS techniques and the broad scope of analytical needs, it may be difficult to decide which type of mass spectrometer is the optimal fit for a given laboratory. Laboratory objectives such as high sensitivity, high resolution, or general-purpose flexibility must be prioritized.

Representative applications for each type of mass spectrometer are indicated below. Use this chart to help choose the best mass spectrometer for your need.

									
Instrument Name		LCMS-8060 LCMS-8050 LCMS-8040 LCMS-8030	LCMS-2020	LCMS-IT-TOF	GCMS-TQ8040	GCMS-QP2010 Ultra	GCMS-QP2010 SE	MALDI-7090 AXIMA Resonance AXIMA Performance	AXIMA Confidence AXIMA Assurance
Ionization Method	EI				●	●	●		
	CI				●	●			
	NCI				●	●			
	ESI	●	●	●					
	NanoESI			●					
	APCI	●	●	●					
	APPI			●					
	DUIS	●	●						
	MALDI							●	●
Mass Spectrometer	Quadrupole	●	●		●	●	●		
	Ion Trap			●				● (Resonance only)	
	TOF			●				●	●
MS	MS	●	●	●	●	●	●	●	●
	MS/MS	●		●	●			●	▲ (PSD only)
	MS <sup>n</sup>			●				● (Resonance only)	
Main Applications		Qualification and quantitation	Qualification and quantitation	Qualification and structural analysis	Qualification and quantitation	Qualification and quantitation	Qualification and quantitation	Qualification and structural analysis	Qualification



LCMS-8060  
LCMS-8050  
LCMS-8040  
LCMS-8030

LCMS-2020

LCMS-IT-TOF

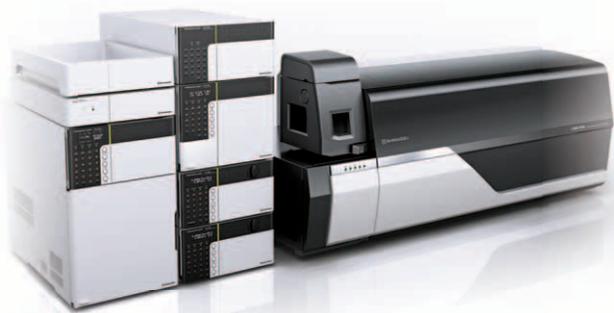
GCMS-TQ8040  
GCMS-  
QP2010 Ultra  
GCMS-  
QP2010 SE

MALDI-7090  
AXIMA  
Series

Environmental	Atmosphere	Benzene, trichloroethylene, tetrachloroethylene, dichloromethane, etc.					●	
	Soil	Trichloroethylene, tetrachloroethylene, dichloromethane, etc.					●	
	Water	Pesticides, PFOS/PFOA, algae bloom toxin, shellfish toxin, etc.	●	●	●	●		
Foods	Ingredient analysis	Amino acids, sugars, catechins, vitamins, etc.	●	●	●	●		
	Additives	Colorings, antibacterial agents, etc.	●	●	●	●		
	Residual pesticides	Insecticides, disinfectants, herbicides, etc.	●	●	●	●		
	Toxins	Mycotoxins, etc.	●	●	●	●		
Life Science/ Pharmaceuticals	Genomics	DNA, RNA						●
	Proteomics	Proteins, peptides	●		●			●
	Metabolomics	Organic acids, amino acids, lipids, etc.	●		●	●	●	
	Synthetic compounds	Low-molecular-weight compounds, antibiotics, antibacterial agents, natural medicines, steroids, etc.	●	●	●	●		
	Impurities	Pharmaceutical impurities, etc.	●	●	●	●		
	HTS	Candidate compounds, etc.		●				
	Pharmacokinetics	Metabolites, etc.	●	●	●	●		
	Toxicity tests	Candidate compounds, etc.	●	●	●			
Drug products	Residual solvents, etc.	●	●	●	●			
Chemistry	Low-molecular-weight organic molecules	Surfactants, antioxidants, fullerenes, etc.	●	●	●	●		●
	Polymer composition analysis	Polymers, rubber, plastics, etc.	●		▲*	●		●
	Additives	Plasticizers, etc.	●	●	●	●		●
	Impurities	Organic impurities, etc.	●	●	●	●		
Clinical Research	Monitoring pharmaceuticals	Pharmaceuticals for treatment, etc.	●	●	●	●		
	Endocrinology research	Hormones, etc.	●	●	●	●		
	Toxicology	Acutely toxic substances, etc.	●	●	●	●		
	Biomarker discovery	Organic low-molecular-weight molecules, peptides, etc.	●		●	●		●
Forensics	Doping testing	Steroids, etc.	●		●	●		
	Identification of target substances	Abused substances, etc.	●		●	●		

\* Primary structural analysis, excluding calculations of average molecular weight, degree of polymerization, and degree of dispersion

# LCMS-8030/8040/8050/8060 Software



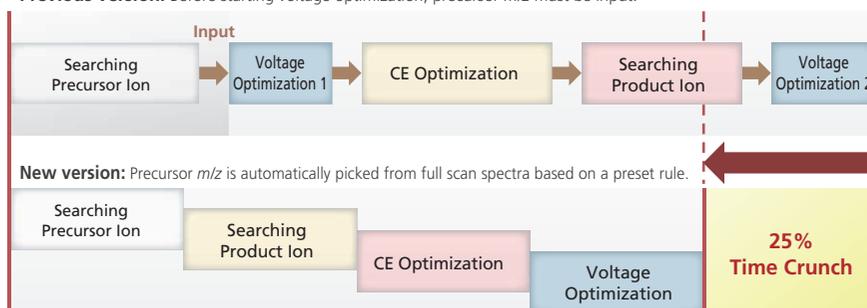
## LabSolutions LCMS

By combining our own thinking with critical inputs from end users we have designed new tools for LabSolutions LCMS software for the LCMS-80 series. LabSolutions LCMS keeps improving its functionalities to deliver you better and more productive workflow.

## Fully Automated MRM Optimization

New MRM optimization function fully automates necessary steps for MRM optimization by seamlessly connecting precursor ion finding on the existing MRM voltages wizard. Furthermore, using overlapping injection capability, approximately 25% time reduction per compound is achieved.

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



## Synchronized Survey Scan

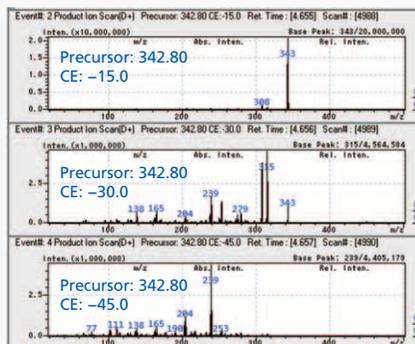
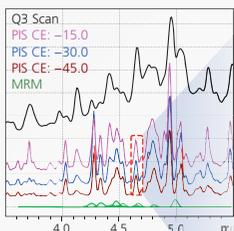
Shimadzu proprietary Synchronized Survey Scan (SSS) automatically performs a product ion scanning whenever a pre-set survey scan threshold is exceeded. For survey scan, either MRM or full scan are applicable. It is very effective data acquisition mode especially for screening application which you want to get quantitative results with higher confidence.

In this example, we have conducted the multiple time segmented MRM measurement with full scan dependent product ion scanning with three different collision energies in entire elution time. The new functionality in SSS now allows different collision energies to be applied to same precursor ion for product ion scanning significantly enhancing qualitative workflows. That means you can use a product ion scan to seek unknown compounds you did not list on MRM events. The improvement of scan sensitivity in LCMS-80 series proposes you a new way for untargeted screening.

Type	Event #	+/-	Compound Name <i>m/z</i>	Time (1.000 min - 7.000 min)
Q3 Scan	1	+	100.00 - 500.00	
Product Ion Scan	2	+	> 20.00 - 500.00	
Product Ion Scan	3	+	> 20.00 - 500.00	
Product Ion Scan	4	+	> 20.00 - 500.00	
MRM	5	+	Atropine 290.15>124.15, 290.15	
MRM	6	+	Bromovalerylurea 223.00>179.	
MRM	7	+	Lidocaine 235.00>86.10, 235.00	
MRM	8	+	Risperidone 411.20>191.05, 411.	
MRM	9	+	Haloperidol 376.15>165.15, 376.	
MRM	10	+	Flunitrazepam 314.05>268.15	
MRM	11	+	Nimetazepam 296.05>250.20, 2.	
MRM	12	+	Estazolam 295.05>267.15, 295.	
MRM	13	+	Triazolam 343.05>308.20, 343.0	

Full scan  
-Product ion scan

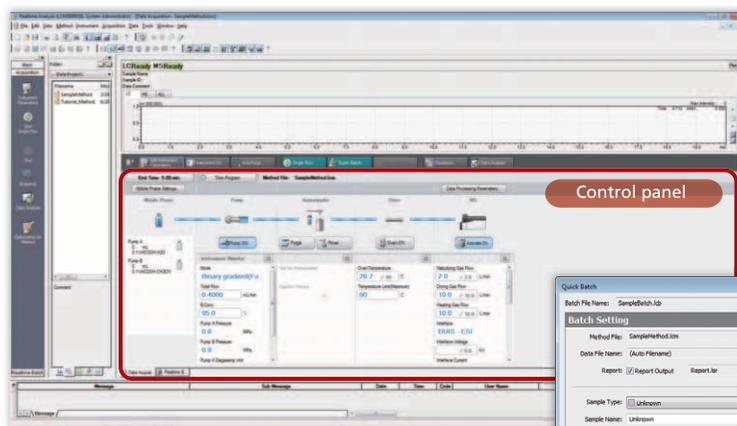
Timed MRM events



# Intuitive User Interface

LabSolutions is empowered by newly designed graphical interface. In method edit window, the GUI with analytical flow line and intuitive icons for each key elements is added. It helps you a lot for the method development and understanding system status. The new functionality, Quick batch incorporates auto-sampler tray

with vial position and three color codes includes standard: sky blue, unknown: purple and control: yellow. You can create new sample queue with higher confidence than previous version of LabSolution software. Previous style is also available in this version. You can switch the setting easily.



## Method development

Graphical user interface with analytical flow line and intuitive icons illustrate each modules require the parameter setting helps a lot for method setting and system monitoring.

## Quick Batch

Streamlines sample submission. A simple color coded autosampler graphic helps to visualize the sample queue quickly. Three color codes have been designed for standards (sky blue), unknowns (purple) and controls (yellow).



# LC/MS/MS Method Package and MRM Library

We know your headache against method development. We have various type of Ready-to-use method packages as well as MRM libraries cover very wide application range.



	Description	Flyer code
Method Package	Residual Pesticides	C146-E160
	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
MRM Library	Cell Culture Profiling	C146-E279
	Metabolic Enzymes in Yeast	C146-E275

# LCMS-2020 Software



## LabSolutions LCMS

LabSolutions LCMS offers integrated LCMS system control and data processing.

Shimadzu's family of instrument software, including LabSolutions LCMS, LCsolution, GCsolution, and GCMSsolution, allows easy operation of analytical instrumentation including tuning, setting method conditions, viewing or analyzing data, and preparing reports.

A mass spectrometer can be operated with the ease of use common to absorption or fluorescence HPLC detectors.

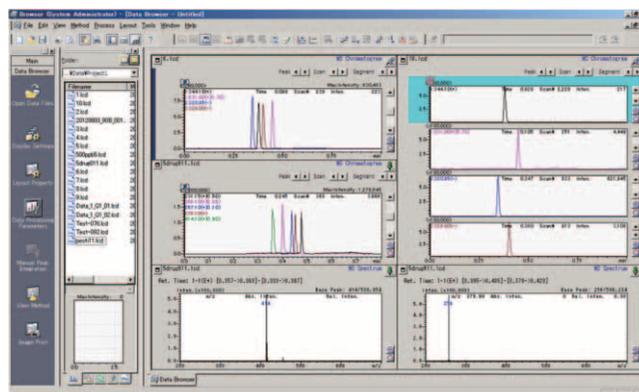
## Data Browser

The data browser allows detection of peaks, analysis of multiple data sets, and comparison of chromatograms and spectra, all in one window.

The extensive and intuitive user interface supports rapid processing of even large data sets.

MS, PDA, and LC chromatograms can be tiled side-by-side or overlaid for easy comparison.

Highly flexible reporting functions allow the creation of specific formats tailored to analytical operations, including chromatograms, calibration curves, quantitative results, and summary reports.

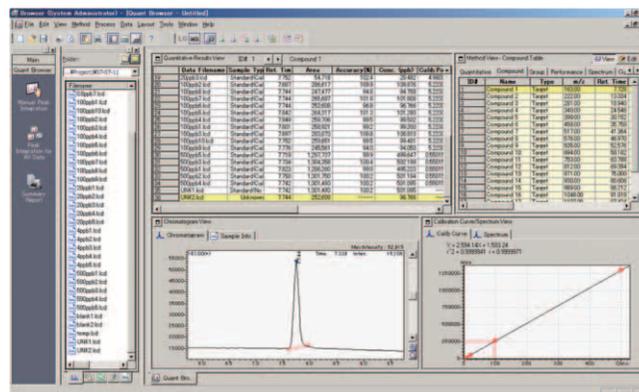


## Quantitation Browser

The quantitation browser has four views: a [Quantitative Results View] for displaying the quantitative calculation results for each set of data, a [Method View] for displaying processing parameters, a [Chromatogram View] for displaying chromatograms and sample information, and a [Calibration Curve/Spectrum View] for displaying the calibration curves and spectra for compounds.

By editing a single method file, the data processing parameters in that method can be used to perform quantitative calculations on multiple sets of data.

Quantitative calculation results for up to 1,024 data files acquired using the same method file can be reviewed and processed together.



# Open Solution Analytical

Open Solution Analytical software is the open access software for LC/LCMS systems. After log-in, submit a sample and perform the analysis on the same screen as sample registration. The progress of the analysis and queue time are shown in the Sample Log-in window for easy verification of the system status.

After the data acquisition is finished, the software automatically sends an e-mail with a URL to a qualitative results report in the Data Browser, allowing chemists to check their results remotely. The user has full functionality – even adding or deleting a peak of a LC or PDA chromatogram.

Launch the Data Browser and review results from any PC connected to the networks. There is no need to install any specialized software on each PC.

A built-in software function allows a user to automatically wash the flow line after each sample analysis, even when using multiple LC columns, to prevent damage to or contamination of the LC column. An additional feature makes it possible to set a specific timeframe or day of the week to start up the system in preparation for analysis.



# ASAPrep

ASAPrep (Automated Scale-up from Analytical to Preparative) provides a unique solution to automate and optimize the purification process and enhances productivity in compound purification and isolation of pharmaceutical drug development.

An open access workflow helps analysts to simply select a pre configured analytical LC/PDA/MS method, submit their sample for analysis, and review the results.

Subsequently, the generic analytical LC data are automatically processed and checked for co-elution or partial separation. A color coded results table helps to accelerate decisions.



# LCMS-IT-TOF Software



## LCMSsolution

LCMSsolution is the workstation software package used to control the LCMS-IT-TOF mass spectrometer and any associated data processing.

Because the software was designed in conjunction with other chromatography products in mind, it can be easily operated by both new users and those users familiar with our other software packages. It ensures that users can access necessary features, like auto-tuning and automatic MS/MS functions, seamlessly and efficiently.

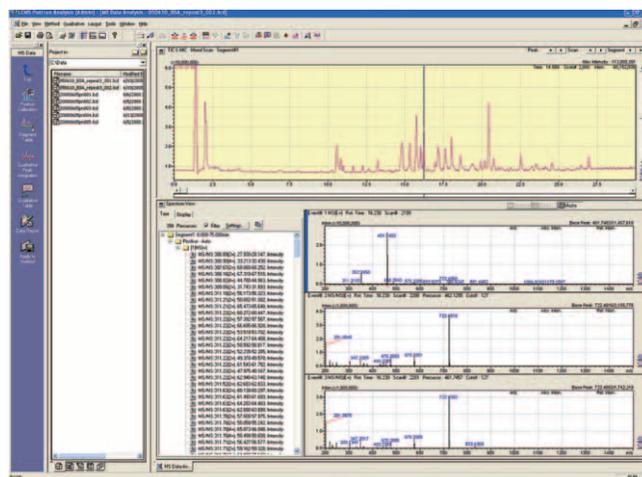
## Data Processing

The data processing functions in the software package are used to quickly analyze the high-throughput and high-accuracy data obtained from the LCMS-IT-TOF system. Processing data using the software is easy and efficient.

The Data Browser function allows loading and viewing up to 64 sets of data at one time.

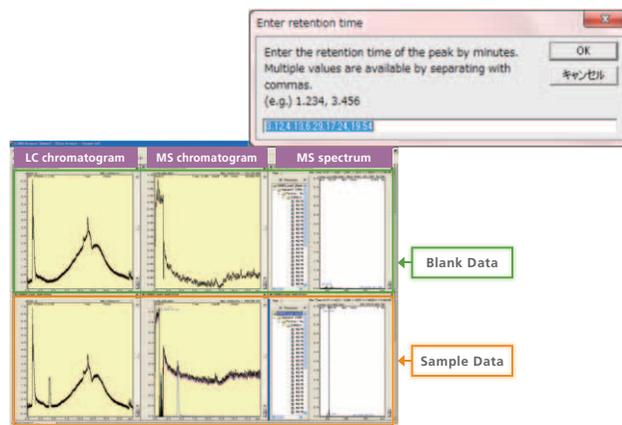
Files can be managed using intuitive operations.

The Quantitation Browser enables simultaneous data processing of multiple sets of data files acquired using a single method. This allows for users to develop logical workflows and faster data processing.



## Trap-Free 2D LC/MS Impurity Identification System

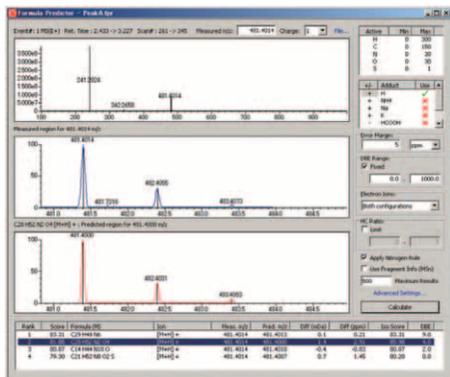
With the use of a 2D LC-LCMS system, no additional method development is required because mobile phases can be changed online. A support tool makes creating a time program and batch schedule easy. The optimal valve sequence can be constructed by entering the retention times for impurity peaks observed in the first-dimension UV chromatogram, and then a batch schedule can be created to acquire data on multiple impurities and their respective blanks. Using the data browser makes identification of impurities easy. In addition, the data browser function allows easy comparison of the details and differences between sample data and blank data, enhancing the efficiency of the impurity identification process.



Example of sample data and blank data displayed in the data browser

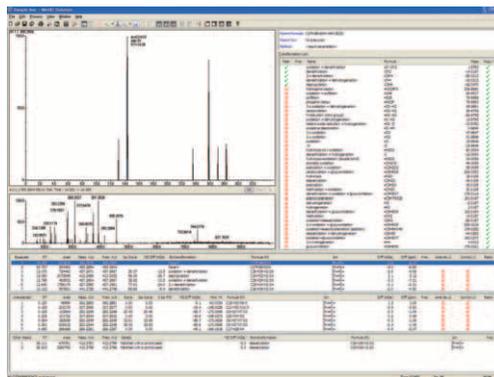
## Formula Predictor

The Formula Predictor software is used to help predict the chemical structure of a target peak by utilizing a proprietary method that narrows down the number of possible chemical formula for a peak of interest.



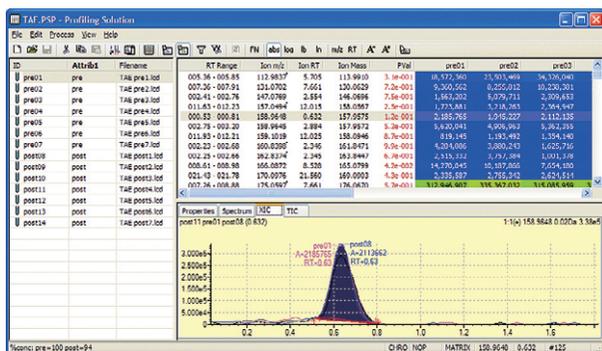
## MetID Solution

This software compares data from samples both before and after they are metabolized, allowing the user to search for expected and unknown metabolites.



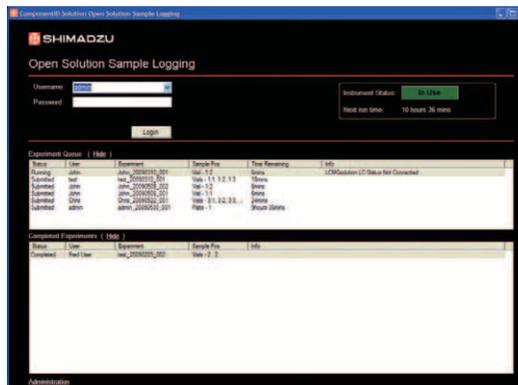
## Profiling Solution Ver.1.1

This data viewer enables multi-file processing and exporting of data for use in commercial multivariate analysis software. Some additional features allow for the correction of retention times and normalization of mass accuracy and signal intensity.



## Open Solution ComponentID

Built for the LCMS-IT-TOF system, this easy-to-use software package allows users, without detailed software knowledge, to perform sample analysis.



## MS Spectra Library for Glycosphingolipids

The main content of the library is gangliosides, which are increasingly targeted for research. It contains the data of 21 ceramides, 193 acidic glycolipids and 42 neutral glycolipids (a total of 256 species). Library searching supports the use of the exact mass of a precursor ion as a search cue, facilitating quick identification of detected glycolipids.



## GC/MS Databases

Shimadzu offers a variety of databases to simplify analysis. The GCMS Smart Database Series is comprised of separate databases for analyzing pesticides, forensic toxicological substances, metabolites and environmental pollutants. The software series supports simultaneous high-sensitivity analysis of samples using GC-MS/MS, eliminating the need to configure complicated analysis conditions. Other databases enable quick screening for residual pesticides in foods; fast identification of forensic toxicology related compounds; and reliable confirmation of hazardous chemicals.

	<b>Database for Quantitation</b> Optimized analytical conditions are registered in the database, enabling analysis to start quickly	<b>Database for Screening</b> The database enables rough quantitation analysis with calibration curves registered in the database
 Pesticides	<b>Smart Pesticides Database</b>	<b>Quick-DB GC/MS Residual Pesticides Database</b>
 Illegal Drugs, Psychotropics, Medicines	<b>Smart Forensic Database</b>	<b>GC/MS Forensic Toxicological Database</b>
 Metabolites	<b>Smart Metabolites Database</b>	
 Semi Volatile Organic Compounds	<b>Smart Environmental Database</b>	<b>Compound Composer Database Software Ver. 2</b>

## Mass Spectral Libraries

 General	<b>NIST Mass Spectral Library</b> <b>WILEY Mass Spectral Library</b>
 Drug	<b>GC/MS MPW DRUG Library</b>
 Pesticide	<b>GC/MS Pesticide Library</b>
 Flavor	<b>FFNSC 2 GC/MS Flavor and Fragrance Library</b>

# AXIMA MALDI Software



## MALDI Solutions

MALDI Solutions™ is the completely new software interface for the MALDI-7090 MALDI TOF-TOF mass spectrometer. Providing a powerful range of tools for method development, acquisition, data processing and interpretation, MALDI solutions has been designed for ease of use and reliability. Each function within the MALDI Solutions suite is targeted to a particular application such as LC-MALDI, tissue imaging or manual control creating a simple and versatile application-centric platform. Coupling the MALDI-7090 with MALDI Solutions provides a stable, high-throughput multi-user system that is ideally placed to meet the demands of modern research laboratories.

## LAUNCHPAD™

LAUNCHPAD™ software controls and processes data from MALDI-TOF MS (AXIMA series) systems.

## Data Acquisition

For more varied applications or rapid investigation of samples, the MALDI-7090 can be operated with a full manual approach. This provides the freedom to explore samples using the full extent of all the acquisition modes: MS, MS/MS, positive and negative ionization.



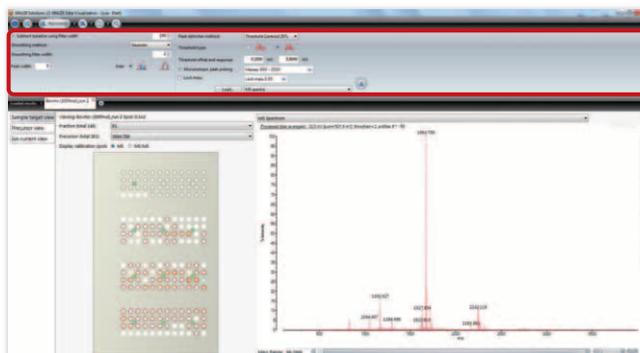
## Data Analysis

The peak processing function allows the user to select from several types of settings from a drop-down list, ranging from a simple settings window to a more detailed one, based on the user's experience.

Seamless integration with many optional software programs ensures smooth data analysis.

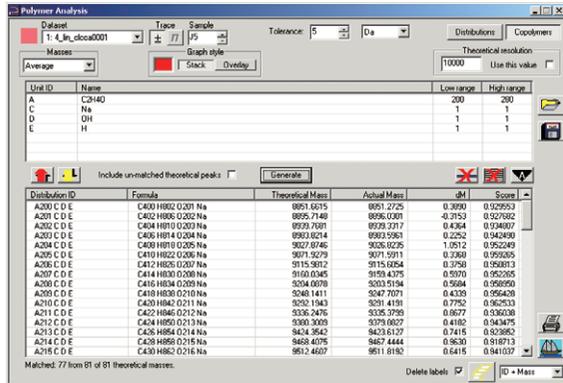
In addition, analytical data can be exported in a variety of formats to allow further analysis using third-party software. Batch processing is also possible.

Optional protein identification software can perform MALDI-MS, MS/MS analyses, and Mascot® search automatically.



## Polymers

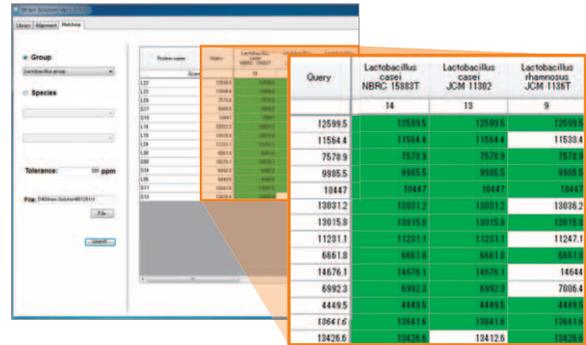
This software is used to analyze both homopolymers and complicated copolymer compounds.



Supported by LAUNCHPAD

## Strain Solution

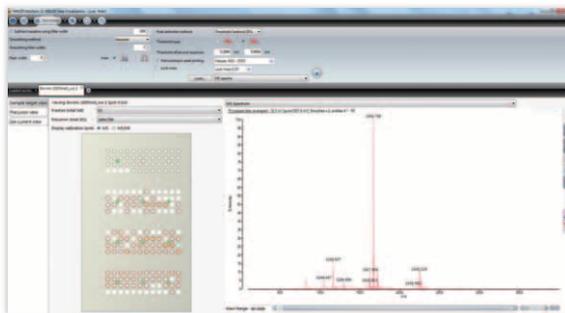
Using the iD<sup>plus</sup> Microorganism Identification System with Strain Solution software enables a theoretical-based molecular phylogenetic classification solution that provides better discrimination capabilities than 16S rRNA gene sequencing.



Supported by LAUNCHPAD

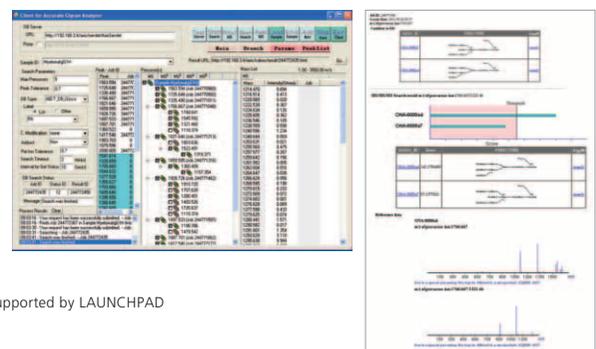
## LC-MALDI

LC-MALDI, MS acquisition, data-dependent MS/MS analysis and protein database identification are fully automated through the LC-MALDI module in MALDI Solutions to maximize protein identifications from even the smallest of sample amount.



## Software for Accurate Glycan Analyzer 2

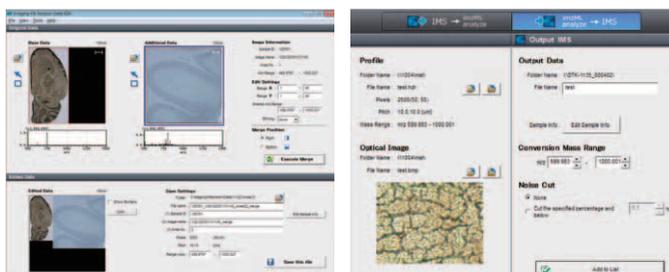
Used in combination with an AXIMA Resonance system, this software identifies glycan structures with distinguishing structural isomers.



Supported by LAUNCHPAD

## Imaging MS Solution Ver.1.1

This software is especially useful for measuring the distribution of medicines and metabolite products on tissue specimens.



iMLayer

# Systems

## GCMS

### Headspace Analysis System

These systems are used for qualitative and quantitative analysis of substances such as flavorings in foods, odors in chemical products, volatile organic compounds (VOCs) in public drinking water, environmental water, or wastewater, and residual solvents in pharmaceuticals.



### Purge & Trap Analysis System

Purge and trap analysis systems are used to perform highly sensitive measurements of VOCs or moldy odor-causing substances in public drinking water, rivers, groundwater, and so on.

### Pyrolysis System

This system thermally decomposes polymer materials, such as plastics, rubbers and resins, over 500°C and analyzes the resulting pyrolysates with GC/MS. It is used for structural analysis of polymer compounds, such as plastics and rubbers.

The Py-Screener system is designed to screen for phthalate esters in polymers. This screening system consists of a sampling toolkit, special standards, and special software and can be easily operated even by novices.



### Thermal Desorption System

Thermal desorption system is suitable for analysis of low concentration samples such as indoor air pollutants, gases generated from parts/materials, fragrance components, and so on. In addition, the sample tube is easily transported, so it is often used when samples must be collected on site. The TD-20 thermal desorption system includes an autosampler capable of holding up to 48 sample tubes. Therefore, data can be collected during night or weekends by batch processing in automatic operation mode.



### Multi-dimensional GCMS system

A multi-dimensional GCMS system performs separation using two columns that have different characteristics. The system has a mechanism in which the components that are insufficiently separated in the first column are introduced ("heart-cut") to a second, different column. This enables analysis with a level of separation that cannot be attained in conventional single-column analysis.



### GC x GC-MS System

This system employs a pair of GC columns, each containing a chemical phase that is orthogonal to the other, connected in series via a modulator.

Unlike multi-dimensional analysis, this system provides comprehensive 2-dimensional separation across the entire chromatogram by repeatedly injecting samples into the second column.



## Direct Sample Injection System

The DI Probe allows a sample to be introduced directly into the ion source without passing through a GC column. It is an effective technique for obtaining mass spectra of synthetic compounds that do not chromatograph well. A DI system can be incorporated into a standard GC-MS configuration without making any changes to the GC. It is then possible to switch between conventional GC column chromatography and DI analysis without making any hardware changes.



## AOC-6000 Multifunctional Autosampler

The AOC-6000 is compatible with three sample injection methods: liquid sample injection, headspace injection, and solid phase micro extraction (SPME) injection. The sample injection method can be selected to suit the form of the sample and the components subject to analysis. Condition setting and control can be performed using GCMSsolution software. The AOC-6000 and GC/MS analysis conditions are recorded in the data measured, so management of analysis accuracy is easily performed. General analysis conditions are preconfigured, enabling analysis to start quickly.



## LCMS

### ASAPrep Analysis / Preparative System

ASAPrep verifies the retention time of the target compound using analytical-scale LC data. The retention time of the target compound is then used by the ASAPrep algorithm to calculate the focused gradient profile for the preparative-scale separation to deliver the highest purity and recovery of the collected LC fractions.



### 2-Dimensional LC/LCMS-IT-TOF System

The Co-Sense for Impurities system features column-switching technology and is designed specifically for the analysis of impurities.

Existing HPLC methods, such as those using phosphate buffer solutions or ion pair reagents, are first used to identify peaks required for structural analysis while a mobile phase suited for LC-MS work is then used to separate components before introduction to the LC-MS system.



## AXIMA

### SEC-MALDI (LC-MALDI) System

The SEC-MALDI system first separates samples into their components by size exclusion chromatography (SEC), then measures the components using MALDI-TOF MS. This is especially useful for analyzing mixtures containing multiple components, such as synthetic polymers.





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