

Method Package Guidebook



Fast, Easy, Stable

The recent development of high-performance analytical instruments has brought tremendous innovation in a variety of industries. Concurrently, analytical targets are also becoming increasingly varied and analytical conditions are becoming more complex. Improving the efficiency of analysis is essential to performing large numbers of analyses in short periods of time.

Shimadzu "Method Package" allow you to begin performing analyses simply and immediately. The Method Packages offer consistent results regardless of who carries out the analysis, dramatically improving productivity in the laboratory.

Find the perfect Method Package for your laboratory from Shimadzu's ready-to-use solutions in a variety of fields.

What is a Method Package?

Method Package contains ready-to-use analytical conditions and sample pretreatment procedures optimized for Shimadzu mass spectrometers and specific analytical applications. Method Packages enable you to perform simultaneous analysis of multiple compounds efficiently and quickly. Method Packages also support workflow automation by facilitating analysis without needing to investigate separation conditions, optimize MS parameters for each compound, and other complex tasks. Shimadzu has developed various Method Packages tailored to different analytical targets.





Analysis

conditions

Sample adjustment method

Pretreatment program

Industries

Industries where Method Packages play a role. Select the appropriate Method Packages for your specific needs.





Life Science

Food & **Beverages**









Library



Environment





In the life sciences, analytes can be involved in various biological processes, such as metabolism, maintenance, and regulation, and exist in a diverse range of sample matrices such as cells, blood, and urine. Analysis efficiency can be dramatically improved by utilizing a Method Packages tailored to your needs. Method Packages also allow regulated drugs to be analyzed with ease.



Metabolites

Provides ready-to-use methods for over 1900 metabolites



Metabolites Method Package Suite

Provides ready-to-use methods for over 1900 metabolites

This suite allows comprehensive analysis of over 1900 metabolites without the need for investigation of separation conditions, MRM optimization or parameter settings. The range of metabolites spans both hydrophilic and hydrophobic compounds, including amino acids, short-chain fatty acids, sugars, nucleotides, bile acids, and lipids. The suite consists of five LC/ MS/MS Method Packages including ready-to-use methods for the LCMS-8050/8060 series, the LC/MS/MS MRM Library for Phospholipid Profiling, the Smart Metabolites Database™ for GC/MS(GC/MS/MS), and a Multiomics Analysis Package.





Primary Metabolites

IC-MS

Measures principal hydrophilic metabolites comprehensively







Ready-to-use methods for 200 compounds This Method Package enables efficient, simultaneous analysis of a large number of compounds. Optimized LC separation conditions and MS parameters reduce the time and effort expended on method development.

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Life science

Total Solution for Metabolomic Analysis of Endogenous Metabolites Using Exact Mass Database

LC/MS/MS Method Package for Primary Metabolites Ver.3



Simultaneous Analysis of 97 Primary Metabolites By PFPP: Pentafluorophenylpropyl Column

A Multiomics Approach Using Metabolomics and Lipidomics

D/L Amino Acids

Analyzed separately D- and L-amino acids in just 10 minutes without derivatization







Simultaneous Analysis of Chiral Amino Acids Produced by Intestinal Microbiota using LC/MS/MS

Most important amino acids exist as stereoisomers. D- and L- forms of

columns with chiral stationary phases, the D- and L-forms of amino acids

can be analyzed separately. With CR-I(+) elution order is from D- to L-,

mirror image isomers, or enantiomers, are named according to their

activity on polarized light. By using CROWNPAK CR-I(+) and CR-I(-)



Analyzes 39 bile acids and 10 internal standards comprehensively and quickly



LC/MS/MS Method Package Bile Acids Ver. 2

Ready-to-use method This Method Package wa to perform routine analy bile acids, in various mat This Method Package all plasma, urine and feces.







Short Chain Fatty Acids

Analyzes short-chain fatty acids with a pretreatment protocol that includes a derivatization step







LC/MS/MS Method Package for Short Chain Fatty Acids

LC/MS/MS Method Package

and with CR-I(-) the elution order is reversed.

for D/L Amino Acids

Short-Chain Fatty Acids and Organic Acids Targeted for Analysis

Of the short-chain fatty acids produced by intestinal bacteria, acetic acid, propionic acid, and butyric acid are well known, and it has been reported that there are some connections between them and lifestyle-related diseases such as obesity and diabetes. Generally speaking, short-chain fatty acids are highly volatile and highly hydrophilic. This makes it difficult to perform LCMS analysis using a conventional reverse phase system. For that reason, this Method Package targets short-chain fatty acids (C2 to C5) that have been derivatized using 3-nitrophenylhydrazine (3-NPH). After setting MRM transitions, it can be used for the simultaneous analysis (of 22 components), including organic acids related to the central metabolic pathways.



Short-Chain Fatty Acids/Organic Acids in Fecal Specimens from SPF and Antibiotic-Fed Mice

Lipid Mediators

Offers efficient analysis of lipid mediator-related substances with different physical properties



LC/MS/MS Method Package for Lipid Mediators Ver. 3

The Retention Time Correcting Tool available in this version simplifies retention time correction, enabling precise identification of isomers that cannot be distinguished by MRM.

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Life scienc

Ready-to-use method for analysis of 49 Bile Acids

This Method Package was developed to provide users a complete solution to perform routine analysis of selected primary, secondary and conjugates bile acids, in various matrices such as plasma, urine and feces.

This Method Package allows comprehensive analysis of 49 Bile Acids from plasma, urine and feces.

Fast Profiling of 39 Bile Acids in Plasma, Urine and Feces $\,>\,$

Profiling of Bile Acids in Human Plasma



nprehensive Monitoring Method for Analyzing B Lipid Mediator Species

A Method of Simultaneous Analysis for 196 Lipid Mediators and Related Compounds



Phospholipid

Offers comprehensive analysis of major phospholipids and determination of an estimated fatty acid composition

> LC/MS/MS MRM Library for Phospholipid Profiling









Development of a Phospholipid Profiling Method

This MRM library includes two methods: one for phospholipid

includes MRM transitions for up to 867 components.

classification by comprehensive analysis of the main phospholipids in

biological samples, and one for fatty acid composition determination

created using analytical results obtained with the classification method.

The library targets phospholipids containing C14 to C22 fatty acids, and



Quantifies modified nucleosides that are candidate biomarkers for COVID-19 severity



LC/MS/MS Method Package for Modified Nucleosides

This Method Package enables the analysis of 125 compounds in under 20 minutes per sample. Performing analysis separately for each compound group such as amino acids and vitamins makes profiling of cell culture components very laborious, but with this Method Package a large number of culture medium components and secreted metabolites can be analyzed simultaneously.



Steroid Hormones

Provides Sample Pretreatment Protocols and Analytical Methods for Steroid Hormones





for Steroid Hormones

Steroid hormones can be analyzed without having to investigate sample pretreatment or analytical methods

The LC/MS/MS method package for steroid hormones contains LC/MS/MS analytical methods with optimized analytical conditions and MS parameters for analyzing 20 kinds of steroid hormones and corrective substances. The package enables comprehensive analysis of steroid hormones ranging from adrenocortical hormones, such as mineralocorticoid and glucocorticoid, to sex hormones, such as androgens, estrogens, and progestogens. The instruction manual also describes examples of pretreatment protocols that include derivatization for blood serum



Reactive Sulfur Profiling

Sample Pretreatment Protocols and Analytical Methods for 17 Sulfur-Containing Metabolites, Including Reactive Sulfur Species



LC/MS/MS Method Package for Reactive Sulfur Profiling

This LC/MS/MS Method Package for Reactive Sulfur Profiling offers analytical methods for LC/MS/MS that target all 17 sulfur-containing metabolites, including reactive sulfur species, with separation conditions and MS parameters that are optimized for each compound. It also comes with example pretreatment protocols, including derivatization steps, for biological samples containing cells and blood plasma. The method package allows the user to analyze sulfur-containing metabolites without time-consuming investigation into sample preparation and analytical conditions. The Shimadzu Multi-omics Analysis Package also offers a tool to visualize quantitative results obtained with this method package. The tool helps users interpret results by providing easy-to-understand graphical displays of the relationships and ratios between metabolic components in different sample sets.









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Simultaneous Analysis Conditions for 125 Compounds





Simultaneous Analysis of 20 Steroid Hormones and High-Sensitivity Analysis of Estrogens



Cell Culture Profiling

Measures a wide range of culture medium components with analytical conditions optimized for culture medium analysis







Complete Analytical Method for the Quantitation of Modified Nucleosides Which is a Candidate Biomarker for COVID-19 Severity

This Method Package provides optimized analytical conditions, including chromatographic separation and MS parameters, for the determination of two types of modified nucleosides and factors for normalization. It also includes examples of sample preparation methods for blood serum and urine samples. Consequently, this product can be used to analyze specific modified nucleosides in urine and blood serum without the need for timeconsuming method development.



Sugars and Sugar Nucleotides

Pretreatment protocols and analytical methods specifically for sugars and nucleotide sugars







Sugars and sugar nucleotides can be efficiently analyzed by minimizing pretreatments and method considerations

The LC/MS/MS Method Package for Sugars and Sugar Nucleotides includes LC/MS/MS analytical methods with analytical conditions and MS parameter settings optimized for analyzing 25 different sugars, amino sugars, sugar acids and sugar alcohols, 9 different sugar nucleotides, related metabolites, and internal standards. In addition, the instruction manual includes examples of pretreating culture media, supernatants, and intracellular metabolites from cultured cells.







Optimized separation conditions and MS parameters for sulfated disaccharides derived from six important glycosaminoglycans.



LC/MS/MS Method Package for Glycosaminoglycans

The LC/MS/MS Method Package for Glycosaminoglycans contains LC/MS/MS analytical methods with optimized separation conditions and MS parameters for sulfated disaccharides derived from six important glycosaminoglycans. It also has example sample preparation protocols for blood spots, including enzymatic preparation. This method package can be used to analyze glycosaminoglycans while saving significant time in the development of sample preparation and analytical protocols.



Pharmaceutical Elemental Impurities

Offers efficient analysis of elemental impurities in drugs by EDX

100ppm~		10ppm~ 1		ppm~	0.1ppr	0.1ppm~	
21	22	23	24	as	²⁶	27	28
Sc	Ti	V	Cr	Mn	Fe	Co	Ni
»	∞	41	a	۹	44	45	46
Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd
\$7-71	л	n	74	75	»	n	78
*	Hf	Ta	W	Re	Os	Ir	Pt
89-103	104	¹⁰⁵	106	¹⁰⁷	¹⁰⁸	100	110
**	Rf	Db	Sg	Bh	Hs	Mt	Ds

La Ce Pr Nd Pm Sm Eu Gd







index



Life science

Pharmaceuticals Impurities Analysis Method Package



This package provides analysis methods to support the four elements in Class 1 as stipulated by ICH Q3D, the three elements in Class 2A, and five elements from among the Class 2B elements. Analysis is performed by creating a calibration curve with a specified standard mixture solution and solutions made by diluting it.

> ICH Q3D Elemental Impurities Analysis of Drug Substances by EDX



Rapid Toxicology Screening

Offers simultaneous analysis of prohibited drugs, sleeping pills, and other common analytes in the forensic field





DPiMS[™]-8060 Method Package for Rapid Toxicology Screening Ver.2

Simple pretreatment for blood and urine samples in only 2 minutes

With the DPiMS-8060, time-consuming pretreatment steps associated with forensic samples are almost completely eliminated. Begin analysis after only simple dilution and centrifugation steps. The DPiMS-8060 is therefore extremely well-suited for mass analysis via rapid screening.





Screening and Semi-Quantitation by LC/MS/MS in Whole Blood Using Rapid Tox Screening

LC/MS/MS Rapid Toxicology Screening System Ver.3



Recommended Solution Guides

Lipid and Fatty Acid Analysis Solutions

Lipids are one of the four major biological substances, along with proteins, carbohydrates, and nucleic acids. Fatty acids are also important in living organisms and make up cell membranes (examples: phospholipids, sphingolipids, cholesterol esters). Both play essential roles in the physiology of living organisms, serving as structural components of biological membranes, mediators of energy storage, and signaling molecules within and between cells. This guidebook highlights key application examples for lipid and fatty acid analysis using various instruments.

Industrial web site for Lipidomics

Introducing a wide range of analysis examples using highly sensitive and rapid analytical instruments that target a wide variety of lipids.

Metabolic Pathway Analysis Solutions

Metabolic pathways are the chain of chemical and enzymatic reactions that occur within a cell in living organisms to support their life. They are a series of reaction pathways that include intermediates from reactants to products. This guidebook introduces applications for metabolic pathway analysis using various instruments.

Life science











Method Packages are effective in the food and beverage field where analytes are derived from various foods and beverages and analytes must be investigated in different ways. Method Packages facilitate rapid simultaneous analysis of multiple components regulated in various countries.



Residual Pesticide

Widely covers residual pesticides regulated in various countries





LC/MS/MS Method Package for Residual Pesticide Ver. 3

■ Database compatible with LabSolutions Connect[™], a tool that automates MRM tuning and optimization

Encompasses the components listed in the Japanese Multiresidue Method for Agricultural Chemicals by LC/MS. Compatible with the components subject to the Chinese GB standards Compatible with the components subject to (EC) Directive No. 396/2005 Contains 6557 MRM transitions for 836 components.



Covers pesticides on the Positive List System that can be analyzed by GC/MS



The method files contained in this package are pre-registered with optimized analytical conditions and compound information, allowing users to start analysis of multiple component samples without having to perform troublesome tasks. Also, information for 542 pesticides that can be batchanalyzed in accordance with the Positive List System is pre-registered.









Pretreatment program for improving the peak shape of polar pesticides

■ Easy data analysis with LabSolutions Insight[™], a powerful data mining and analytics program

GC/MS Method Package Ver.2 for Residual Pesticides in Foods



Method for the determination of 182 Residual



Veterinary Drugs

Offers rapid analysis of veterinary drug compounds



LC/MS/MS Method Package for Veterinary Drugs Ver. 2



Method Package including 129 veterinary drug compounds, more than 3 times as many as Ver. 1

High-speed method with just 16.5 mins detection time Pretreatment program to improve the peak shape for polar veterinary drug

compounds Data analysis is made simple with LabSolutions Insight™





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Compounds using MRM Spectrum Mode

Aminoglycoside Antibiotics

A simultaneous quantitative analysis solution for all regulated aminoglycoside antibiotics







LC/MS/MS Method Package for Aminoglycoside Antibiotics

Complete method for fast quantitative screening of 13 aminoglycosides in meat, eggs and milk.

Increase identification confidence with MRM Spectrum mode and

LabSolutions Insight[™] Screening.

No ion-pairing reagent required.

Includes single sample preparation protocol usable for meat, eggs and milk.



Mycotoxins

Offers simultaneous multi-component analysis of mycotoxins regulated in various countries



LC/MS/MS Method Package for Mycotoxins

the USA, the EU, and China.

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Dioxins

Complies with EU regulations on dioxins in foods



EU Regulation Compliant GC-MS/MS Method Package for Dioxins in Foods

Supports the Analysis of Dioxins in Foods Using GC-MS/MS

The analysis of dioxins in foods was mainly performed using magnetic sector (double-focusing) GC-MS instruments. However, in June 2014, the GC-MS/MS method was officially recognized in the EU as being equivalent to the magnetic sector GC-MS method (EU 589/2014). This product consists of method files for the analysis of dioxins in foods, and a report creation tool, supporting the analysis of dioxins via GC-MS/MS.











kins	in	Foods	and	Feeds	with	BEIS



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Total Solution for Metabolomic Analysis of Endogenous Metabolites Using Exact Mass Database

Short Chain Fatty Acids

Analyzes short-chain fatty acids with a pretreatment protocol that includes a derivatization step

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LC/MS/MS Method Package for Short Chain Fatty Acids

Short-Chain Fatty Acids and Organic Acids Targeted for Analysis

Of the short-chain fatty acids produced by intestinal bacteria, acetic acid, propionic acid, and butyric acid are well known, and it has been reported that there are some connections between them and lifestyle-related diseases such as obesity and diabetes. Generally speaking, short-chain fatty acids are highly volatile and highly hydrophilic. This makes it difficult to perform LCMS analysis using a conventional reverse phase system. For that reason, this Method Package targets short-chain fatty acids (C2 to C5) that have been derivatized using 3-nitrophenylhydrazine (3-NPH). After setting MRM transitions, it can be used for the simultaneous analysis (of 22 components), including organic acids related to the central metabolic pathways.



Shimadzu provides total support for food safety, whether it is farm to fork or bait to plate. As a leading manufacturer of a wide range of analytical instruments, Shimadzu undertakes development of new instruments and technologies, and provides comprehensive service support in order to keep up with changing market demands.

i-Series Food Safety Analyzer Screening of 24 Synthetic Antimicrobial Compounds That

Antimicrobial Screening System

Detects Synthetic Antimicrobial Agents of the Standard Residual Concentration with High Sensitivity

Mycotoxin Screening System

EU Criteria Concentrations of 10 Mycotoxin Components Detected with High Sensitivity in Only 14 Minutes



Specimens from SPF and Antibiotic-Fed Mice













In the environment field, the safety of our lived environment is a primary focus, including pesticides in our food and surroundings, water quality, and textiles. Method Packages are effective because the parameters being tested vary by analyte and by the conditions of each analyte. Method Packages facilitate rapid simultaneous analysis of multiple components regulated in various countries.





Residual Pesticide

Widely covers residual pesticides regulated in various countries

LC-MS





■ Database compatible with LabSolutions Connect[™], a tool that automates MRM tuning and optimization

Encompasses the components listed in the Japanese Multiresidue Method for Agricultural Chemicals by LC/MS. Compatible with the components subject to the Chinese GB standards Compatible with the components subject to (EC) Directive No. 396/2005 Contains 6557 MRM transitions for 836 components.



Covers pesticides on the Positive List System that can be analyzed by GC/MS



The method files contained in this package are pre-registered with optimized analytical conditions and compound information, allowing users to start analysis of multiple component samples without having to perform troublesome tasks. Also, information for 542 pesticides that can be batch-analyzed in accordance with the Positive List System is pre-registered.







LC/MS/MS Method Package for Residual Pesticide Ver. 3



Pretreatment program for improving the peak shape of polar pesticides

■ Easy data analysis with LabSolutions Insight[™], a powerful data mining and analytics program

Determination of 313 Residual Pesticides in Black tea >

GC/MS Method Package Ver.2 for Residual Pesticides in Foods



Determination of 326 Residual Pesticides in Rice

Residual pesticides in Carrotoleoresin

Water Quality

Enables simultaneous multi-component analysis of golf course pesticides and pesticides subject to water quality regulations





Ready-to-Use Methods Provided

Shimadzu provides method files, including pre-registered MRM parameters with optimized quantitative and reference ions, LC separation parameters, and retention times and peak identification parameters for each compound, as well as report templates for outputting quantitation results, as a package. If retention times are adjusted when the system is introduced, based on the HPLC configuration delivered, the analysis process can be started as soon as the specified columns, mobile phases, and standard samples are supplied.



Analyze plastics that are degraded or altered by exposure to UV rays or heat



Plastic Analyzer Method Package

The Plastic Analyzer Method Package includes an FTIR spectral library for plastics degraded by UV rays and heat. Utilizing searches of this library demonstrates its effectiveness in the analysis of unknown samples that are difficult to identify with standard libraries. Examples include plastics degraded by exposure to UV rays as well as contaminants and defective items altered by heating.





Textiles

Allows comprehensive identification of hazardous substances regulated by international standards and self-regulated by manufacturers



LC-MS

In recent years, while many issues have been raised related to food safety and the environment, the safety of textiles, which are indispensable for everyday life, has become a particular concern. Countries throughout the world, and especially in the EU, are regulating and investigating hazardous chemicals in textiles. Additionally, regulations have been tightened with respect to hazardous chemicals in textiles. This includes the adoption of the OEKO-TEX[®] Standard 100, a globally consolidated, independent examination and authentication system for textiles, and the implementation of voluntary regulations by various manufacturers. In addition to the currently regulated components, this Method Package provides analysis methods covering the major compounds in the OEKO-TEX[®] Standard 100 and voluntary regulations by various manufacturers.





PFAS

Analyzes organofluorine compounds in drinking water according to EPA methods 533 and 537.1





LC/MS/MS Method Package for PFAS in Drinking Water

Provides Methods for Analyzing Per- and Polyfluoroalkyl Substances in Drinking Water According to EPA Methods 533 and 537.1

The United States Environmental Protection Agency (US EPA) has standardized two methods for the analysis of Per- and Polyfluoroalkyl Substances (PFAS) in drinking water: EPA Method 537.1 and 533, encompassing a total of 29 PFAS. These methods were used as reference for creating a vetted LC/MS/MS Method Package for Analyzing PFAS in Drinking Water. This method package includes ready-to-use analytical conditions for EPA Methods 533 and 537.1, examples of analytical procedures for the methods, and various other information, such as precautions for sample preparation and analysis. Using this product, 52 PFAS compounds* in drinking water can be analyzed.





Per- and Polyfluoroalkyl Substances (PFAS)

Best Practices for Optimizing PFAS Analysis









LC/MS/MS Method Package for Restricted Chemicals in Textiles



Various restricted chemicals in textiles can be detected.

Analysis of Ikylphenol Ethoxylates (APEO) and Alkylphenols (AP)





Method Packages are effective in the chemicals and materials field, where analytes are a wide variety of chemically synthesized components and substances found in textiles, plastics, and other materials. Method Packages enable rapid simultaneous analysis of multiple components regulated in various countries.



Plastics

Analyze plastics that are degraded or altered by exposure to UV rays or heat



The Plastic Analyzer Method Package includes an FTIR spectral library for plastics degraded by UV rays and heat. Utilizing searches of this library demonstrates its effectiveness in the analysis of unknown samples that are difficult to identify with standard libraries. Examples include plastics degraded by exposure to UV rays as well as contaminants and defective items altered by heating.





Textiles

Allows comprehensive identification of hazardous substances regulated by international standards and self-regulated by manufacturers



Phthalate Esters and Brominated Flame Retardants

Offers rapid simultaneous analysis that also supports phthalate ester testing for REACH regulations





Making the Difficult simple

Py-Screener[™] Ver. 2 is designed to screen for brominated flame retardants, such as PBBs and PBDEs, and phthalate esters in polymers. These substances are regulated under the Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS (II) Directive) in Europe. The pyrolyzer GC/MS (Py-GC/MS) is used to selectively detect and quantify these restricted substances thermally extracted from samples. This screening system consists of a sampling toolkit, special standards, and special software and can be easily operated even by novices.





for Restricted Chemicals in Textiles

LC/MS/MS Method Package

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Analysis of Ikylphenol Ethoxylates (APEO) and Alkylphenols (AP)







24











Evaluation of Effectiveness of Dedicated High Durability Column

Useful tools

Utilize these software together with Method Package

Multi-Analyte Quantitation Software LabSolutions Insight[™]



Faster Data Review for Dramatically **Higher Productivity**

Mass spectrometry laboratories can acquire thousands of chromatograms per day. Insight provides tools to streamline data review and focus on the chromatograms that need critical attention. Insight automatically applies your peak detection criteria to data and flags any deviations, allowing you to analyze data more efficiently.

Learn more

LC/MS,GC/MS Data Analysis Software **Multi-omics Analysis Package**



Peak Processing Optional Software for LabSolutions Insight™ **Peakintelligence**[™]



Peakintelligence is a world-first^{*1} algorithm incorporating AI assistance to search for chromatography peaks. Having learnt peak processing skills from experienced users, the AI can process data with the same skill level. The algorithm can be implemented immediately without adjusting any parameters.*2

*1 As of August 2019, from internal research *2 The algorithm cannot learn from the user's peak data

Learn more for LC-MS

Learn more for GC-MS

Multivariate Analysis Software That Supports MRM Data

Traverse MS



The Multi-omics Analysis Package is metabolic engineering software that can automatically generate metabolic maps and perform a variety of data analysis based on the vast amounts of mass spectrometry data generated in fields such as metabolomics, proteomics, and flux analysis. In conjunction with the various Method Package and databases offered by Shimadzu for metabolomic analysis, the Multi-omics Analysis Package can help increase the efficiency of metabolomic data analysis work. The intuitive visualization of data provides powerful support for drug discovery, functionally-enhanced foods, bioengineering, and other life sciences research applications.

Learn more



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 statistically analysis for metabolic pathway analysis.

Note: The software is a product of Reifycs Inc.

Learn more



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