C10G-E094

SHIMADZU
Excellence in Science

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.

Industries

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

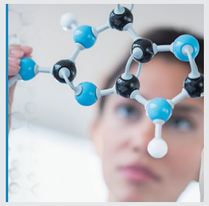
Life science

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

Primary Metabolites

D/L Amino Acids



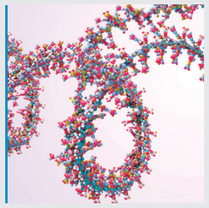
Short Chain Fatty Acids

Bile Acids

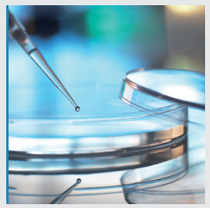
Lipid Mediators

Phospholipid

Modified Nucleosides

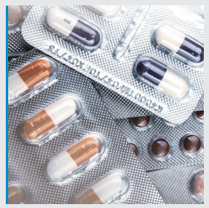


Cell Culture Profiling



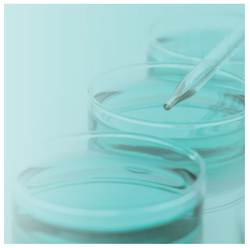
Pharmaceutical Elemental Impurities

Rapid Toxicology Screening



Metabolites

Provides ready-to-use methods for over 1900 metabolites



LC-MS

GC-MS

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 Multi-omics Analysis Package.

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

Primary Metabolites

Measures principal hydrophilic metabolites comprehensively

LC-MS

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

Ready-to-use methods for 200 compounds

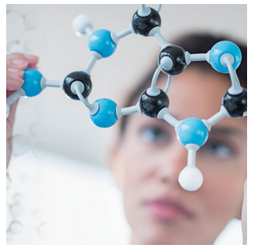
This Method Package enables efficient, simultaneous analysis of a large number of compounds. Optimized LC separation conditions and MS parameters reduce the time and effort expended on method development.

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



LC-MS

LC/MS/MS Method Package for D/L Amino Acids

Most important amino acids exist as stereoisomers. D- and L- forms of mirror image isomers, or enantiomers, are named according to their activity on polarized light. By using CROWNPAK CR-I(+) and CR-I(-) 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-, and with CR-I(-) the elution order is reversed.

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

Short Chain Fatty Acids

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

LC-MS

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

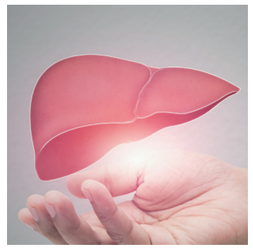
Short-Chain Fatty Acids and Organic Acids Targeted for Analysis

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.

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

Bile Acids

Analyzes 39 bile acids and 10 internal standards comprehensively and quickly



LC-MS

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

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

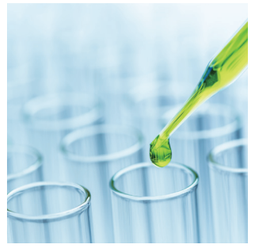
This Method Package was developed to provide users a complete solution to perform routine analysis of selected primary, secondary and conjugates bile acids, in various matrices such as plasma, urine and feces.
This Method Package allows comprehensive analysis of 49 Bile Acids from plasma, urine and feces.

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

Profiling of Bile Acids in Human Plasma

Lipid Mediators

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



LC-MS

LC/MS/MS Method Package for Lipid Mediators

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

Comprehensive Monitoring Method for Analyzing 158 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

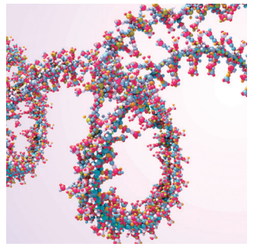
LC/MS/MS MRM Library for Phospholipid Profiling

This MRM library includes two methods: one for phospholipid 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 includes MRM transitions for up to 867 components.

Development of a Phospholipid Profiling Method

Modified Nucleosides

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



LC-MS

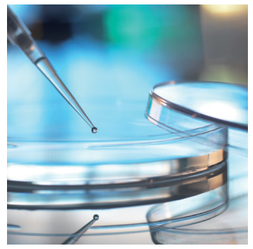
LC/MS/MS Method Package for Modified Nucleosides

Simultaneous Analysis Conditions for 125 Compounds

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.

Cell Culture Profiling

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



LC-MS

LC/MS/MS Method Package for Cell Culture Profiling Ver. 2

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

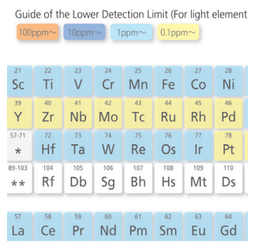
This Method Package provides optimized analytical conditions, including chromatographic separation and MS parameters, for the determination of two types of modified nucleosides and factors for normalization. It also includes examples of sample preparation methods for blood serum and urine samples. Consequently,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

Comprehensive Cell Culture Profiling

Cell Culture Media Analysis Platform: C2MAP System

Pharmaceutical Elemental Impurities

Offers efficient analysis of elemental impurities in drugs by EDX



EDX

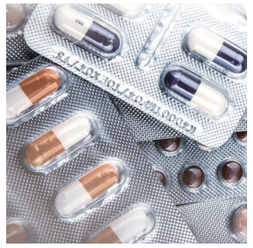
Pharmaceuticals Impurities Analysis Method Package

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



PESI-MS

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

For more information, visit industry website

- Life Science
- Small Molecule Pharma-ceutical
- Bio-pharma-ceutical
- Clinical Research, Forensics

Food & Beverages

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

Veterinary Drugs

Aminoglycoside Antibiotics

Mycotoxins

Dioxins

Metabolites

Short Chain Fatty Acids

For more information, visit industry website

Food and beverages

Residual Pesticide

Widely covers residual pesticides regulated in various countries

LC-MS

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.

- **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

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

GC-MS

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

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.

Determination of 326 Residual Pesticides in Rice

Method for the determination of 182 Residual Pesticides in Milk

Veterinary Drugs

Offers rapid analysis of veterinary drug compounds

LC-MS

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™

Quantitative Analysis of Veterinary Drugs

Multi-Residue Veterinary Drug Analysis of >200 Compounds using MRM Spectrum Mode

Aminoglycoside Antibiotics

A simultaneous quantitative analysis solution for all regulated aminoglycoside antibiotics

LC-MS

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.

Fast Quantitative Analysis of Aminoglycoside Antibiotic Residues in Meat, Eggs and Milk

Mycotoxins

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

LC-MS

LC/MS/MS Method Package for Mycotoxins

Mycotoxins are highly toxic chemical byproducts from fungi commonly found in crops, and residual content in foods are regulated the world over. This Method Package provides simultaneous multi-component analysis conditions for mycotoxins subject to the regulations in Japan, the USA, the EU, and China.

- Mycotoxins in Grain
- Mycotoxin Screening System

Dioxins

Complies with EU regulations on dioxins in foods

GC-MS

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

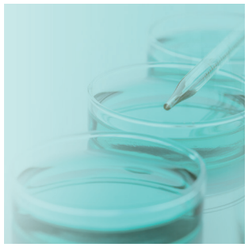
Supports the Analysis of Dioxins in Foods Using GC-MS/MS

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.

- Dioxins in Foods and Feeds
- Dioxins in Foods and Feeds with BEIS

Metabolites

Provides ready-to-use methods for over 1900 metabolites



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

Environment

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 | Water Quality | PFAS | Plastics | Textiles

Residual Pesticide

Widely covers residual pesticides regulated in various countries

LC-MS

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
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■ **Pretreatment program for improving the peak shape of polar pesticides**

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Residual Pesticide

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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

LC-MS

LC/MS/MS Method Package for Water Quality Analysis

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.

PFAS

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

LC-MS

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

Provides Procedure and Method for Analyzing Organofluorine Compounds in Drinking Water According to EPA Methods 533 and 537.1

As various countries implement regulations and assess the presence of PFAS(Per- and Polyfluoroalkyl Substances)s in the environment and drinking water, there is a need to standardize the analytical methods used to quantitatively evaluate PFAS concentrations. This Method Package includes ready-to-use analytical methods and examples of analytical procedures compliant with EPA Methods 533 and 537.1, and various other information, such as precautions for sample pretreatment and analysis.

Per- and Polyfluoroalkyl Substances (PFAS)

Best Practices for Optimizing PFAS Analysis

Plastics

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

FTIR

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.

Microplastics Sampled from Rivers

Plastic Analyzer

Textiles

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

LC-MS

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

Various restricted chemicals in textiles can be detected.

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.

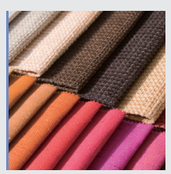
Analysis of lkylphenol Ethoxylates (APEO) and Alkylphenols (AP)

For more information, visit industry website

Environment

Chemical, Material

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.



Textiles

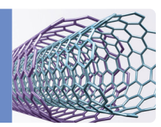
Plastics

Phthalate Esters and Brominated Flame Retardants

For more information, visit industry website

Chemicals

Engineering Materials



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Microplastics Sampled from Rivers

Plastic Analyzer

Phthalate Esters and Brominated Flame Retardants

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

GC-MS

Screening System for Phthalate Esters and Brominated Flame Retardants: Py-Screener Ver.2

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.

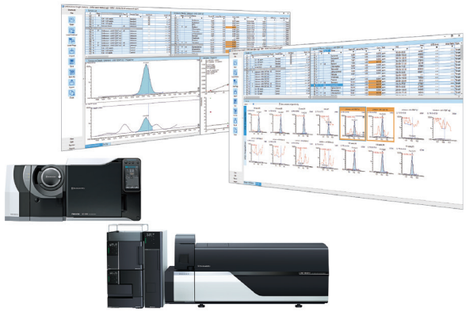
Evaluation of Effectiveness of Dedicated High Durability Column

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

Peak Processing Optional Software for LabSolutions™ LCMS and LabSolutions Insight™

Peakintelligence™

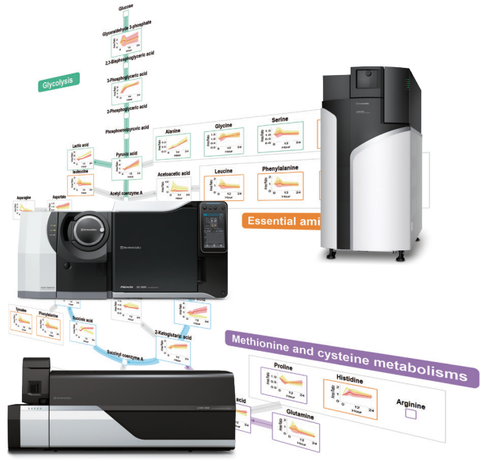
Peakintelligence is a world-first*1 algorithm incorporating AI assistance to search for chromatography peaks. Having learnt peak processing skills from experienced users, the AI can process data with the same skill level. The algorithm can be implemented immediately without adjusting any parameters.*2

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

Learn more

LC/MS,GC/MS Data Analysis Software

Multi-omics Analysis Package

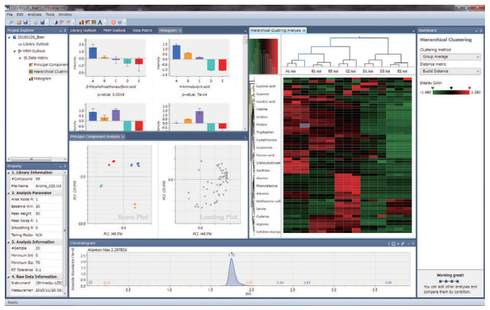


The Multi-omics Analysis Package is metabolic engineering software that can automatically generate metabolic maps and perform a variety of data analysis based on the vast amounts of mass spectrometry data generated in fields such as metabolomics, proteomics, and flux analysis. In conjunction with the 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

Multivariate Analysis Software That Supports MRM Data

Traverse MS



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.

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