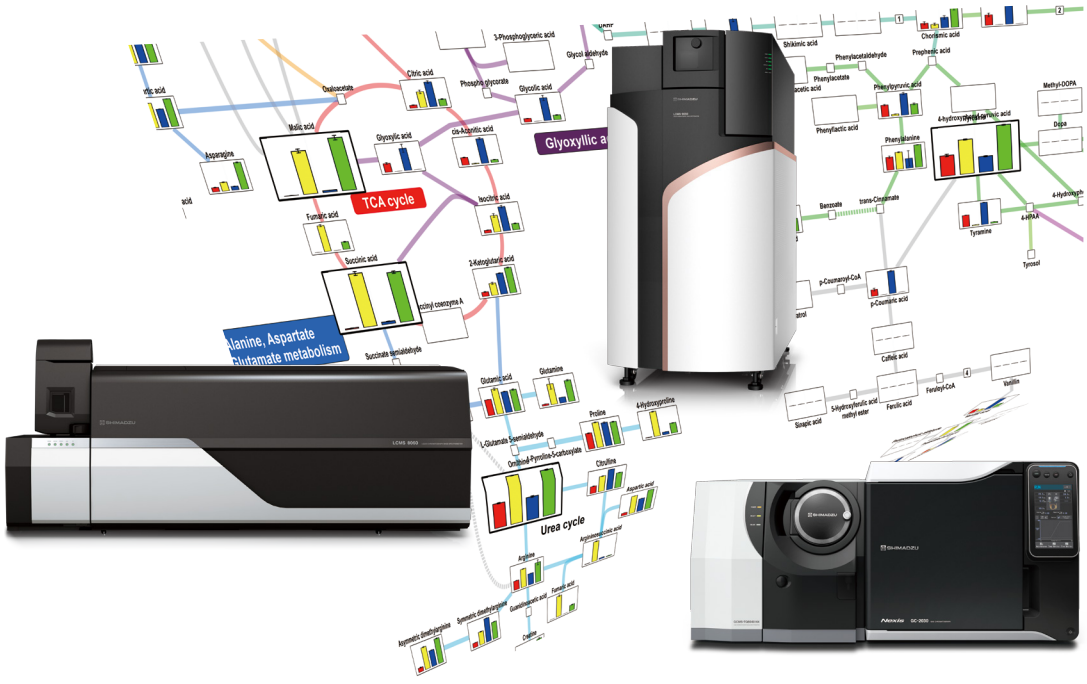
SHIMADZU
Excellence in Science

LC-MS, GC-MS Data Analysis Software

Multi-omics Analysis Package



Multi-omics Analysis Package is metabolic engineering software that can automatically display metabolic maps and perform a variety of data analyses based on the vast amount of mass spectrometry data obtained in metabolomics, proteomics, and flux analysis. In conjunction with the various method packages and databases provided by Shimadzu for metabolomic analysis, it can heighten 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.

Visualize Quantitative Changes in Compounds on a Metabolic Map Using Simple Operations

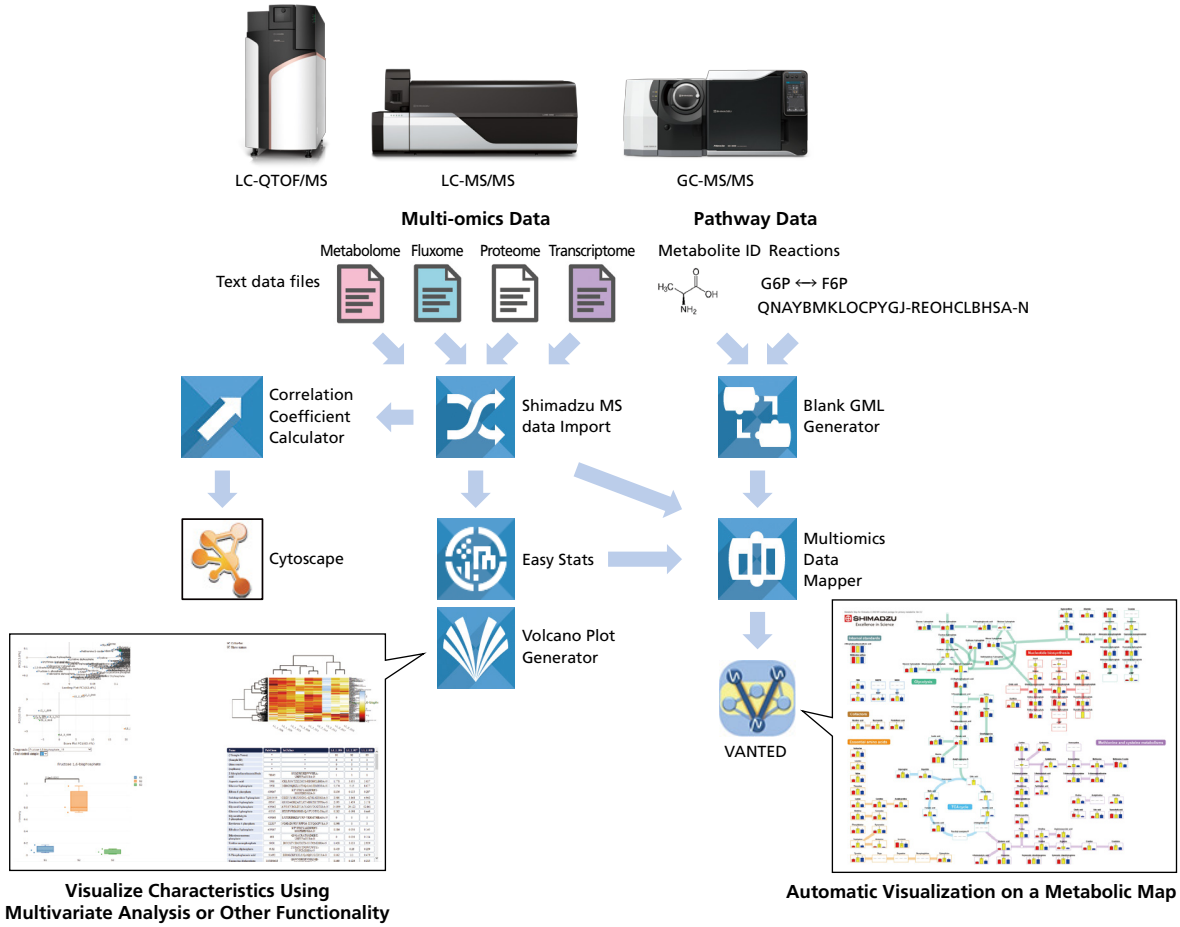
The software dramatically decreases the work of graphing measurement data and projecting it on a metabolic map.

Extract Statistically Significant Compounds Using Simple Operations

It makes it easy to use volcano plots for comparing two groups, principal component analysis (PCA) for comparing multiple groups, hierarchical clustering analysis (HCA), and box plots. PCA, HCA, and box plots can be linked in the same window to conveniently extract significant compounds. Further, the metabolic map can be enlarged to show where the extracted compounds are located, supporting confirmation and interpretation of the data.

Includes Visualization Templates Compatible with a Variety of LC-MS and GC-MS Method Packages

The software is designed to work in combination with various Shimadzu method packages that contain sample pretreatment methods and analytical conditions as ready-to-use methods. This ensures that the entire process from measurement using mass spectrometers to data analysis can be efficiently implemented. The included visualization templates (metabolic maps) are compatible with method packages for LC-MS primary metabolites, lipid mediators and bile acids, and with the GC-MS Smart Metabolites Database™. The templates can be used as is or customized using simple operations.



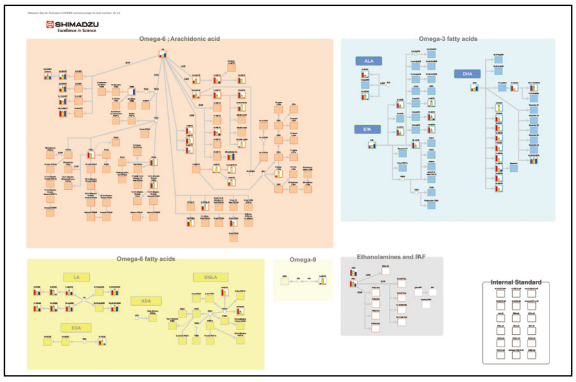
Visualize Characteristics Using Multivariate Analysis or Other Functionality

Automatic Visualization on a Metabolic Map

Click here for an introduction to Multi-omics Analysis Package and instructional videos. >

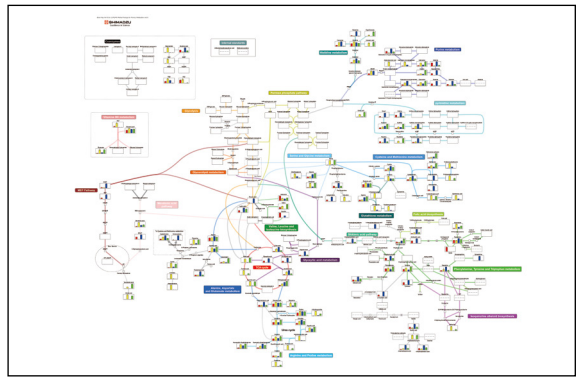
Data Analysis Example

A. Analysis of Temporal Changes in Commercially Available Plasma Using the Lipid Mediators Method Package



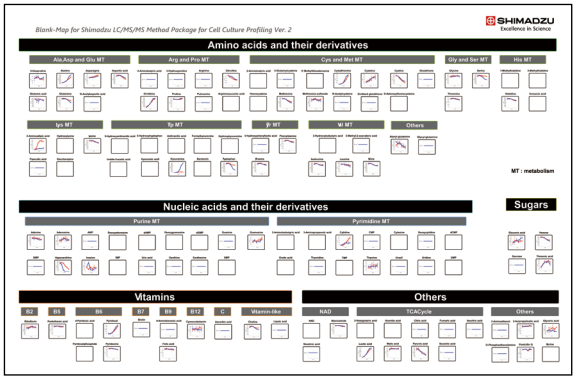
The results of a batch analysis of fatty acids containing eicosanoids in human plasma and serum are easily analyzed by visualization on a metabolic map.
Click here for details. >

B. Comprehensive Analysis of Extracts and Culture Supernatants of E. coli and Yeast Using the Primary Metabolites Method Package



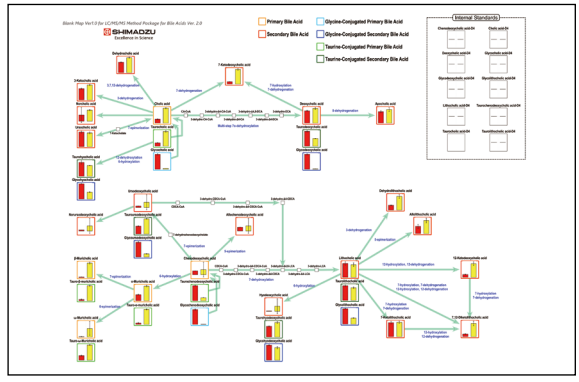
Data analysis and visualization of batch analysis results, including the primary metabolites of E. coli and yeast, support discussions based on metabolic pathways.
Click here for details. (Japanese) >

C. Identification of Time Series Changes in Metabolites in an iPS Cell Culture Supernatant Using the Cell Culture Profiling Method Package



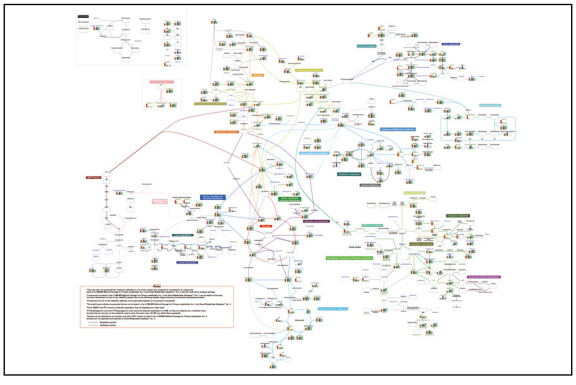
Data analysis and visualization of the batch analysis results of an iPS cell culture supernatant make it possible to search for components that are significantly different across samples.
Click here for details. >

D. Analysis of Metabolites in Mouse Feces and Human Plasma Using the Bile Acids Method Package



High-throughput, low-cost routine analysis is provided by the rapid analysis and visualization of bile acids contained in human plasma and mouse feces.
Click here for details. >

E. LC-MS and GC-MS Analysis of Metabolic Changes in Genetically Mutated Drosophila, and Visualization on a Single Metabolic Map



In order to examine metabolic changes in genetically mutated drosophila in more detail, they were analyzed using both LC-MS and GC-MS. Integration and visualization of both sets of results on a single blank map enable a comprehensive examination of the data.
Click here for details. >

Acknowledgments

A. This metabolic map was developed in cooperation with the Department of Lipidomics, Graduate School of Medicine, The University of Tokyo.

B. The samples were provided by the Engineering Biology Research Center, Kobe University.

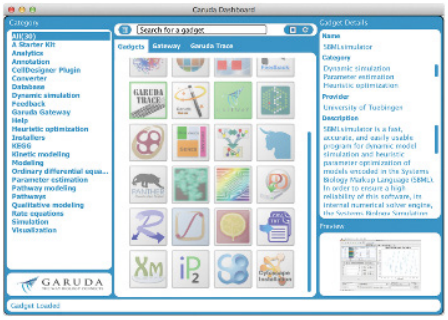
C. The samples were provided by the Foundation for Biomedical Research and Innovation at Kobe.

E. This data was provided by Assistant Professor Kashio at the Graduate School of Pharmaceutical Sciences, The University of Tokyo.

Click here for the latest information on the Multi-omics Analysis Package >

Tools for Data Analysis

The Multi-omics Analysis Package was developed based on tools (gadgets) released on the GARUDA open research platform, which is managed primarily by The Systems Biology Institute (SBI).



http://www.garuda-alliance.org/

Data Analysis Tools Used in the Multi-omics Analysis Package

Volcano Plot

This tool combines a t-test (for statistically significant differences) and a fold-change (example: differences in mean values such as 2 times or 1/2) to visualize the differences between two groups. The Volcano Plot gadget developed by Shimadzu is included in this package.

EasyStats

This tool is for visualizing principal component analysis (PCA) and hierarchical cluster analysis (HCA) results, and box plots (including t-tests) of measurement data. Metabolite data analysis results can be checked in a single window, enabling the comprehensive determination of characteristic changes.

VANTED

This tool is maintained by the University of Konstanz in Germany for the visualization and data analysis of networks across different data sets. GARUDA support was developed at Monash University in Australia. It supports metabolite profiling and the visualization of enzymatic activity data on a metabolic map, and the analysis of biological processes.

Cytoscape

This bioinformatics tool developed by the Cytoscape Consortium is used to visualize metabolic pathways and integrate gene expression profiles with related data. It is especially useful for analyzing networks and visualizing correlations.

Method Packages Supported by Multi-omics Analysis Package*1

Product Name	Catalog No.
Primary Metabolites	C146-E227
Cell Culture Profiling	C146-E408
Lipid Mediators	C146-E381
Bile Acids	C146-E428
Exact Mass Database for Endogenous Metabolites*2	C146-E401
Smart Metabolites Database	C146-E277

*1 Multi-omics Analysis Package is included with LC/MS/MS Method Package, Primary Metabolites, Cell Culture Profiling, and Metabolites Method Package Suite.
*2 Blank maps for visualization are not available for Short Chain Fatty Acids.

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