

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 packages 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.

Visualize Changes in Compound Quantities on a Metabolic Map Using Simple Operations

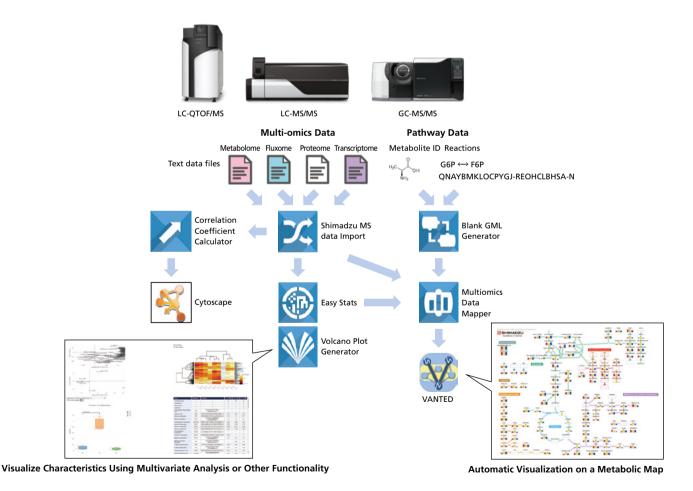
The software dramatically decreases the amount of work required for graphing measurement data or displaying it on a metabolic map.

Identify 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. Linked PCA, HCA, and box plot results can be displayed in the same window to conveniently identify significant compounds. The metabolic map can be enlarged to confirm where identified compounds are located on the map and to support confirming and interpreting the data.

Includes Visualization Template Files Compatible with a Variety of Method Packages

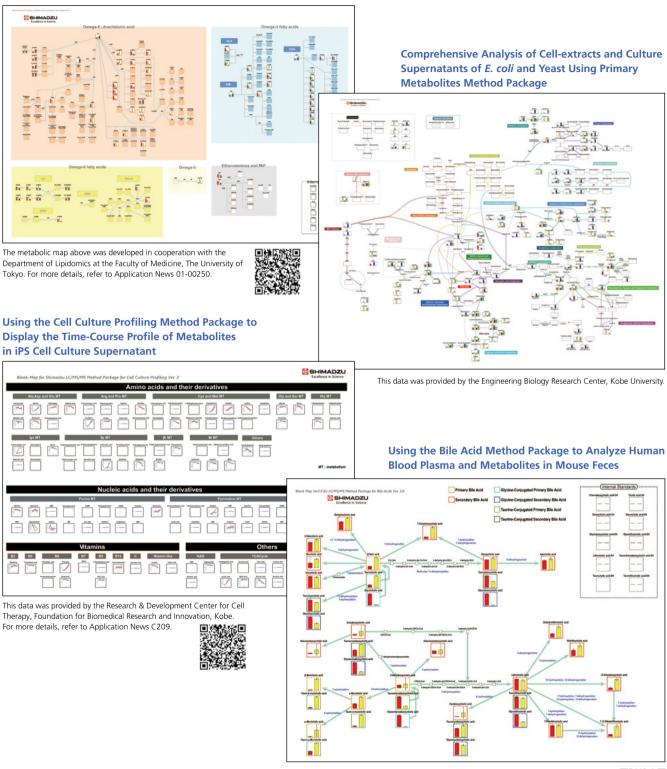
The templates are designed to work in combination with various Shimadzu method packages. These packages contain sample pretreatment methods and analytical conditions for use as "ready-to-use methods," which ensure the entire process, from mass spectrometry analysis to data analysis, can be performed with ease. In particular, these visualization templates (metabolic maps) are compatible with method packages for primary metabolites, cell culture profiling, lipid mediators, and bile acid. The templates can be used as-is or customized using simple operations.





Data Analysis Example

Using the Lipid Mediator Method Package to Display Quantitative Changes in Human Plasma and Serum





For more details, refer to Application News 01-00196.



Tools for Data Analysis

The Multi-omics Analysis Package is based on software tools (called gadgets) that have been released on the GARUDA platform - an open research platform developed by the GARUDA Alliance and led by The Systems Biology Institute, Japan (SBI).



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

Data Analysis Tools Used in the Multi-omics Analysis Package



■ Volcano Plot

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



EasyStats

This tool is for visualizing principal component analysis (PCA) or hierarchical cluster analysis (HCA) results or box plots (including t-test) of measurement data. It can display metabolite data analysis results in a single window to enable comprehensive determination of characteristic changes.



Tool maintained at University of Konstanz, Germany, for visualization and analysis of networks across different data sets. (GARUDA support was developed at Monash University)



Cvtoscape

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

■ LC/MS/MS Method Packages Supported by Multi-omics Analysis Package

Product	Brochure code
Primary Metabolites	C146-E437
Cell Culture Profiling	C146-E408
Lipid Mediators	C146-E381
Bile Acids	C146-E428

^{*} The Multi-omics Analysis Package is included with the LC/MS/MS Method Package for Primary Metabolite, Cell Culture Profiling, and Metabolites Method Package Suite.



GARUDA is a trademark of The Systems Biology Institute.



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