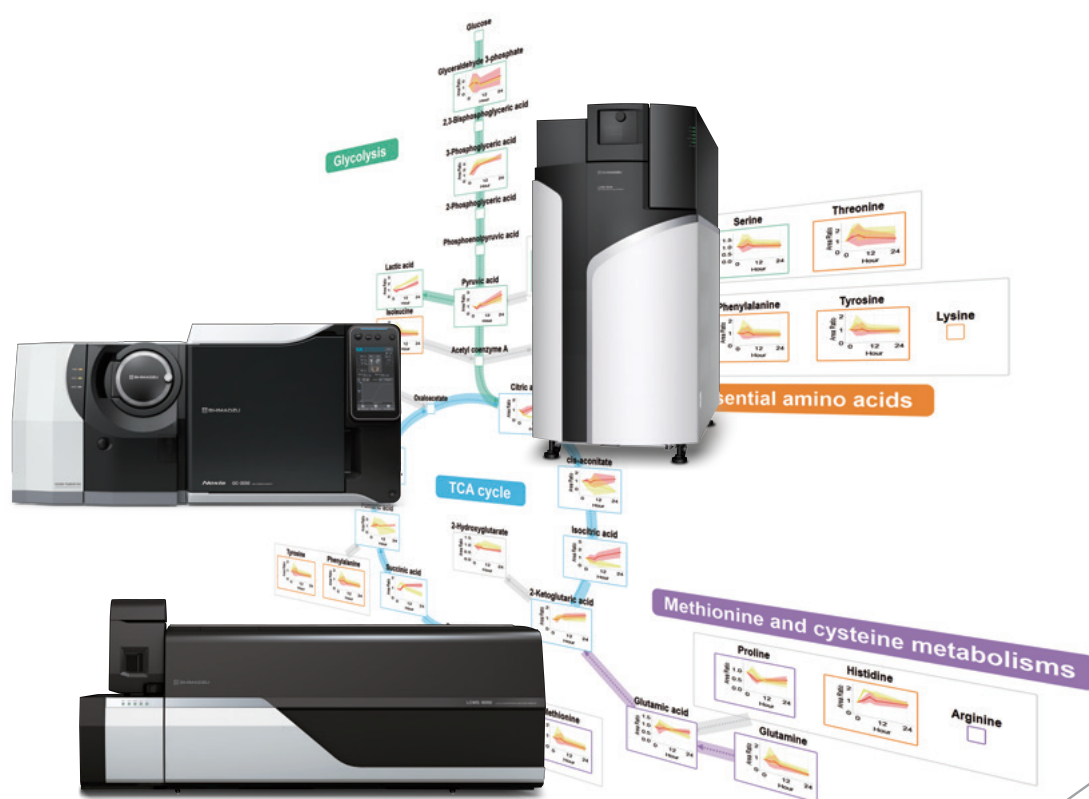# SHIMADZU
Excellence in Science

LC/MS, GC/MS Data Analysis Software

Multi-omics Analysis Package

The Multi-omics Analysis Package, developed for metabolic engineering applications, provides the ability to automatically generate metabolic maps and perform a variety of data analysis for the vast data generated in fields like metabolomics, proteomics and flux analysis. It offers a powerful platform to support drug discovery, bioengineering and other life science research applications.

Automatically Visualize Quantitative Changes in Metabolites and Proteins on a Metabolic Map

Dramatically reduces the amount of work required for bottleneck processes of analyzing and visualizing data, such as displaying data on a metabolic map and analyzing correlations.
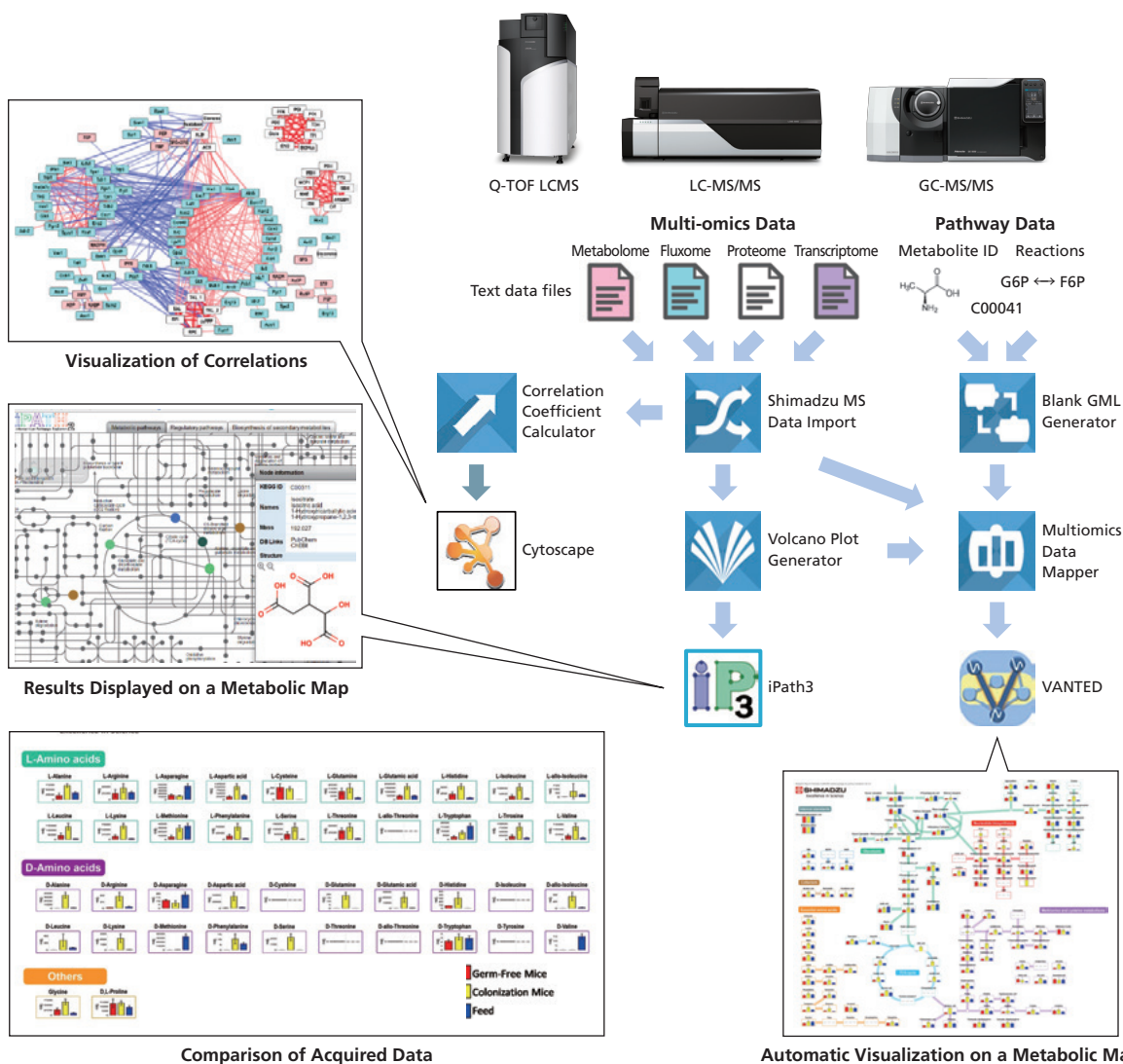
Works Perfectly with Software Developed by the World's Top Research Institutions

In combination with various other software (called gadgets) connected on the GARUDA™ platform, it offers optimal workflows for multi-dimensional analyses.

Integrated Support for Operations from Data Acquisition to Analysis

The software includes various data processing gadgets which connect with corresponding data analysis gadgets, providing a seamless, connected experience of a single software program.

It is designed to work in combination with various Shimadzu databases prepared with "Ready-to-Use Methods" for everything from sample pretreatment to analytical conditions, which ensures the entire process flow, from obtaining mass spectrometer measurements to data analysis, can be performed smoothly.

Visualization of Correlations

Results Displayed on a Metabolic Map

Comparison of Acquired Data

Automatic Visualization on a Metabolic Map

Q-TOF LCMS   LC-MS/MS   GC-MS/MS

Multi-omics Data
Metabolome Fluxome Proteome Transcriptome

Pathway Data
Metabolite ID   Reactions
G6P ⟷ F6P
C00041

Text data files

Correlation Coefficient Calculator

Shimadzu MS Data Import

Blank GML Generator

Cytoscape

Volcano Plot Generator

Multiomics Data Mapper

iPath3

VANTED

Data Analysis Example

Changes in metabolite levels in a cell culture medium over time were measured using a GC-MS system. Acquired data was analyzed using the Multi-omics Analysis Package and metabolite changes were visualized by displaying them on a metabolic map.
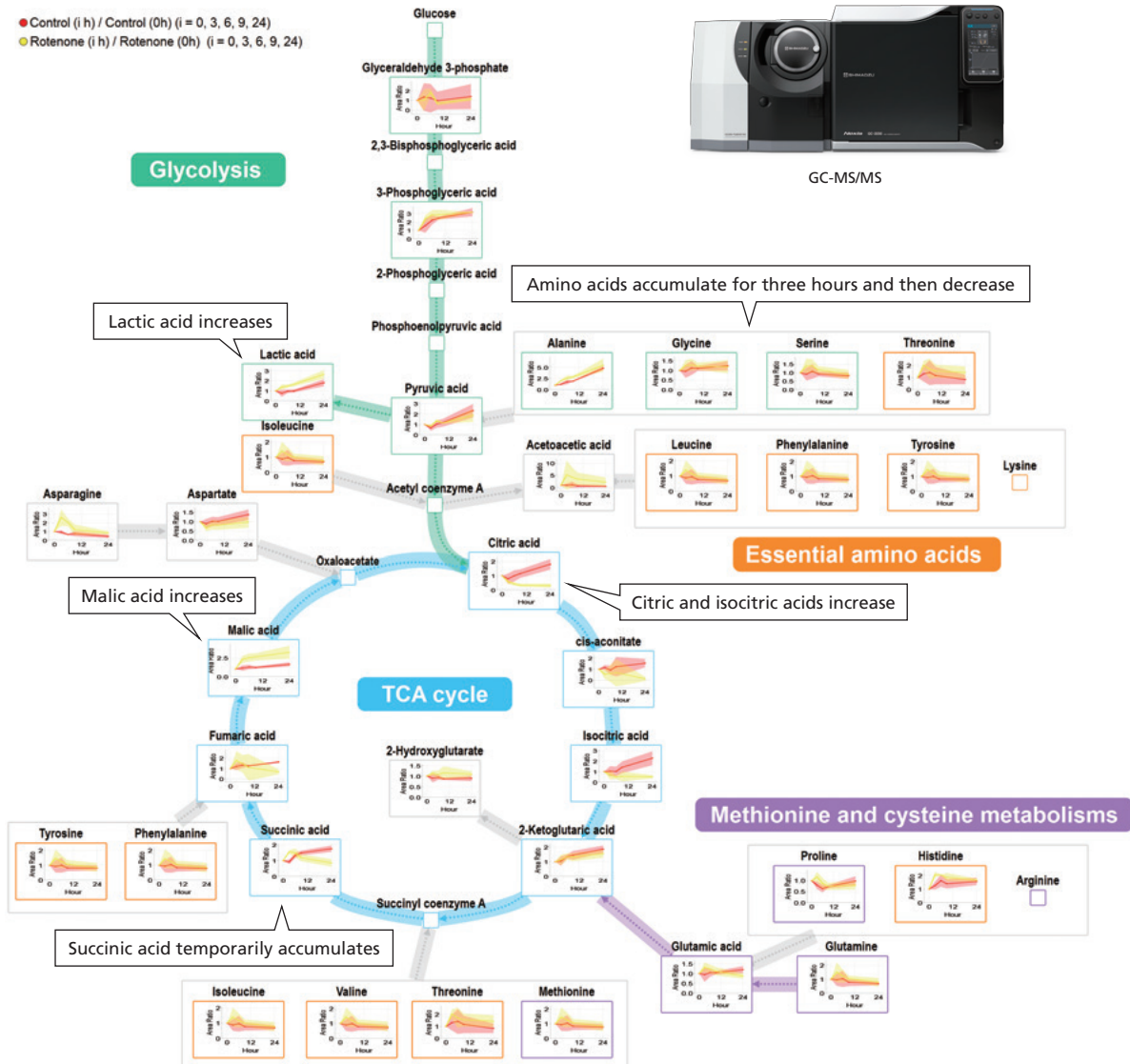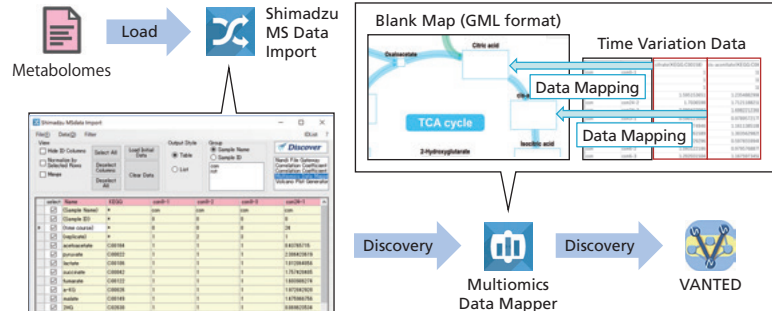
Experiment Protocol

Culture MCF-7 cell line for 15 hours.

▼

Replace culture medium with medium spiked with rotenone.

▼

Collect culture medium after 0, 3, 6, 9, and 24 hours.

▼

Use GC-MS system to measure metabolite quantities.

▼

Analyze data using Multi-omics Analysis Package.

GC-MS/MS

- ● Control (i h) / Control (0h) (i = 0, 3, 6, 9, 24)
- ● Rotenone (i h) / Rotenone (0h) (i = 0, 3, 6, 9, 24)

Glucose

Glycolysis

Glyceraldehyde 3-phosphate

2,3-Bisphosphoglyceric acid

3-Phosphoglyceric acid

2-Phosphoglyceric acid

Phosphoenolpyruvic acid

Amino acids accumulate for three hours and then decrease

Lactic acid increases

Lactic acid

Isoleucine

Pyruvic acid

Alanine · Glycine · Serine · Threonine

Acetoacetic acid · Leucine · Phenylalanine · Tyrosine · Lysine

Acetyl coenzyme A

Essential amino acids

Asparagine · Aspartate

Oxaloacetate

Citric acid

Citric and isocitric acids increase

Malic acid increases

Malic acid

TCA cycle

cis-aconitate

Fumaric acid · 2-Hydroxyglutarate · Isocitric acid

Tyrosine · Phenylalanine

Succinic acid · 2-Ketoglutaric acid

Methionine and cysteine metabolisms

Succinyl coenzyme A

Proline · Histidine · Arginine

Succinic acid temporarily accumulates

Glutamic acid · Glutamine

Isoleucine · Valine · Threonine · Methionine

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 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.

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

■ iPath
Data analysis tool developed by the European Molecular Biology Laboratory that can be used for visualization of diverse metabolic pathways or data mapping and customization.

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

Method Packages for Omics

■ GC/MS, GC-MS/MS Method Package for Metabolites

Description	Flyer code
Smart Metabolites Database™	C146-E277A

■ LC/MS/MS Method Packages

Description	Flyer code
Primary Metabolites	C146-E227A
Short Chain Fatty Acid	C146-E355
Lipid Mediators	C146-E381
D/L Amino Acids	C146-E336
Cell Culture Profiling	C146-E279

■ LC/MS/MS MRM Library

Description	Flyer code
Metabolic Enzymes in Yeast	C146-E275A
Phospholipid Profiling	C146-E314

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GARUDA is a trademark of The Systems Biology Institute.

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