

For LabSolutions LCMS

LC/MS/MS Method Package for Primary Metabolites Ver.2

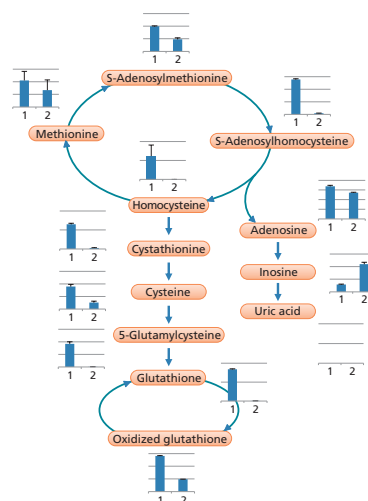


Ready-to-Use Analytical Conditions

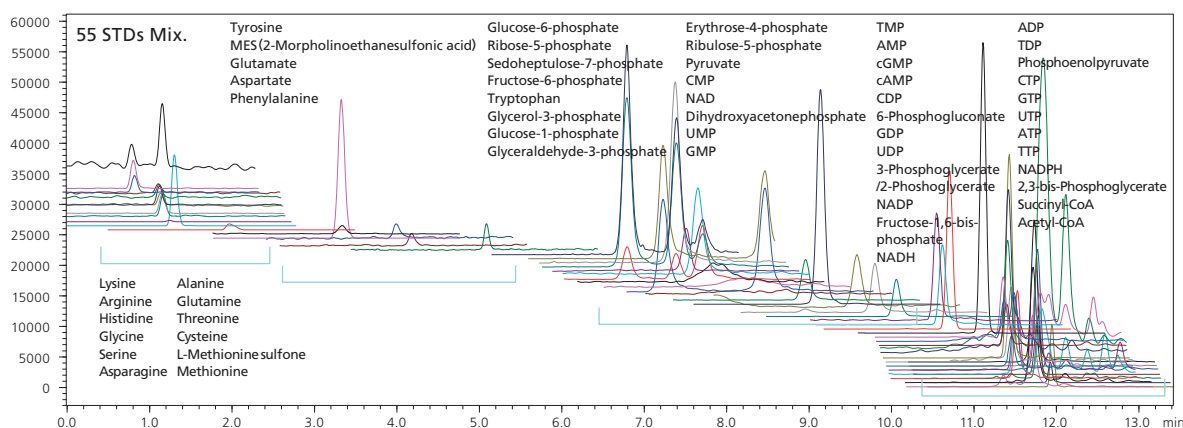
Shimadzu Method Packages deliver conditions for efficient and simultaneous multi-component analysis. They enable the user to quickly and easily implement complex methods without costly and laborious method development by providing sample preparation protocols, LC separation conditions, and MS acquisition parameters.

Two Selectable Analysis Methods

Customers can select an appropriate analysis method from the two methods; analysis using an ion pairing reagent (55 components) and analysis using a PFPP column (97 components) according to the instrument conditions or metabolites to be analyzed.



Area ratio comparison between two tissues
focused on methylation cycle



Overlaid MRM chromatograms for 55 standards mixture by ion pair method

Supporting LCMS-8040/8045/8050/8060

LC/MS/MS Method Package for Primary Metabolites Ver. 2 supports LCMS-8040/8045/8050/8060, enables high-sensitivity simultaneous multi-component analyses of primary metabolites.

Complete from Sample Preparation to Analysis

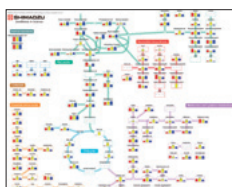
Protocols are included for the preparation of extracts from biological tissue. Saving the user time and money, even laboratories unfamiliar with extraction can follow prescribed steps for LC/MS/MS sample preparation.

Normalization of Multiple Sample Results

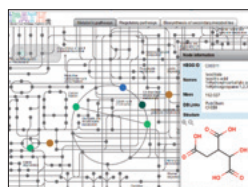
Due to mass differences between biological tissue samples, normalization of results must be performed when multiple samples are analyzed. This method package includes optimized analytical conditions for two internal standards to permit normalization across multiple samples.

Improved Data Analysis Functionality in Method Package

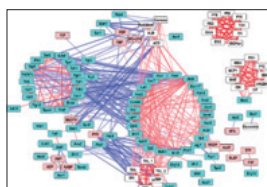
A wide variety of new data analysis functions have been added to the LC/MS/MS Method Package for Primary Metabolites. Functions such as automatically pasting data on metabolic maps, using a bar graph to compare changes in compound quantities, or graphing the changes as a function of time, for example, can be performed using simple operations. It also enables correlation analysis, volcano plots, displaying data on metabolic maps for target compounds, and other functionality. Consequently, it can significantly reduce the amount of work required for bottleneck processes such as data analysis and visualization, so that all operations from measurement to data analysis can be performed smoothly.



Automatic Visualization
on a Metabolic Map



Results Displayed on a
Metabolic Map

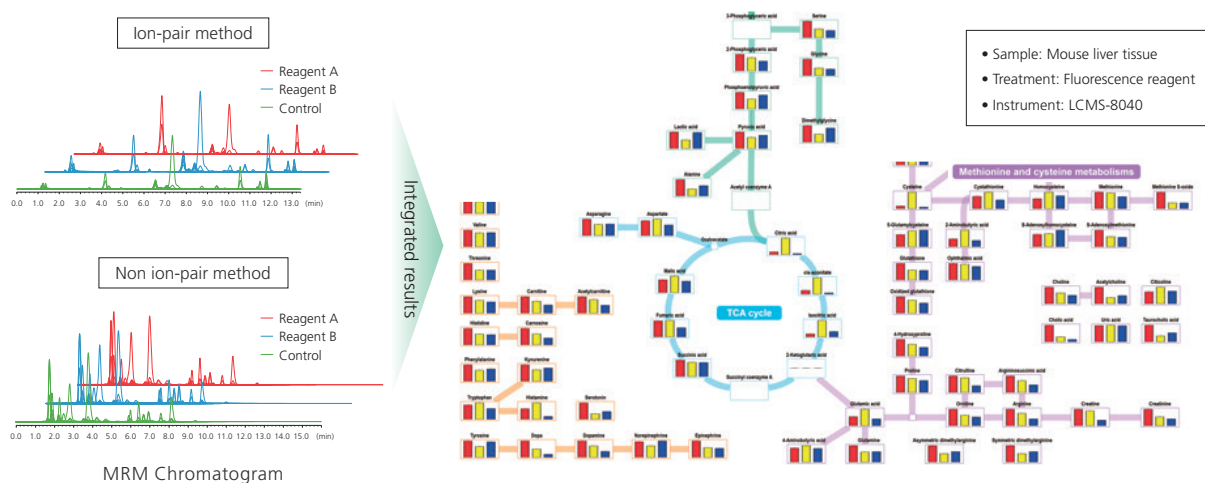


Visualization of Correlations



Comparison of Measurement Data

Data Analysis Example: Visualization of Data on a Metabolic Map



Tools for Data Analysis

In this method package, we provide the data analysis software developed based on tools (gadgets) that have been released on the GARUDA™ open research platform, which is mainly managed by The Systems Biology Institute, Japan (SBI).



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



Data Analysis Tools Used in Method Package



Volcano Plot

A tool that combines a t-test (statistically significant difference) and a fold analysis (Example: Difference in mean value such as 2 times or 1/2) to visualize the differences between the 2 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.

Index of compounds

List of compounds for ion pair method			
Glycolytic system	Nucleotides	Co-enzyme	NAD NADH NADP NADPH
Pentose-phosphate pathway	Nucleotides	Co-enzyme	NAD NADH NADP NADPH
TCA cycle	Nucleotides	Co-enzyme	NAD NADH NADP NADPH
Amino acids	Nucleotides	Co-enzyme	NAD NADH NADP NADPH

* In this method package, customer can select an appropriate analysis method from the two methods using ion pairing reagent (57 components) and PFPP column (97 components) according to the instrument conditions or metabolites to be analyzed.

* The analysis method using ion-pairing reagents is recommended for fluctuation analysis of primary metabolites related to major metabolic pathways such as glycolysis, the pentose phosphate cycle, diphosphate and triphosphate nucleotides. While, the analysis method using PFPP columns is recommended for analysis of amino acids, organic acids (including the TCA circuit), the Methylation cycle and the Urea cycle.

Remarks and Precautions

1. LabSolutions LCMS Ver.5.93 or later is required.
2. Shimadzu makes no warranty regarding the accuracy of information included in the database or the usefulness of information obtained from using the database.
3. It is the user's responsibility to adopt appropriate quality control tests using standard samples to confirm qualitative and quantitative information obtained with this method package.

List of compounds for PFPP column method			
Glycolytic system	TCA cycle	Amino acids	Organic acids
Methylation and Transulfuration cycle	Methylation and Transulfuration cycle	Methylation and Transulfuration cycle	Methylation and Transulfuration cycle

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