C146-E408

SHIMADZU
Excellence in Science

For LabSolutions LCMS

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

Simultaneous Analysis Conditions for 125 Compounds

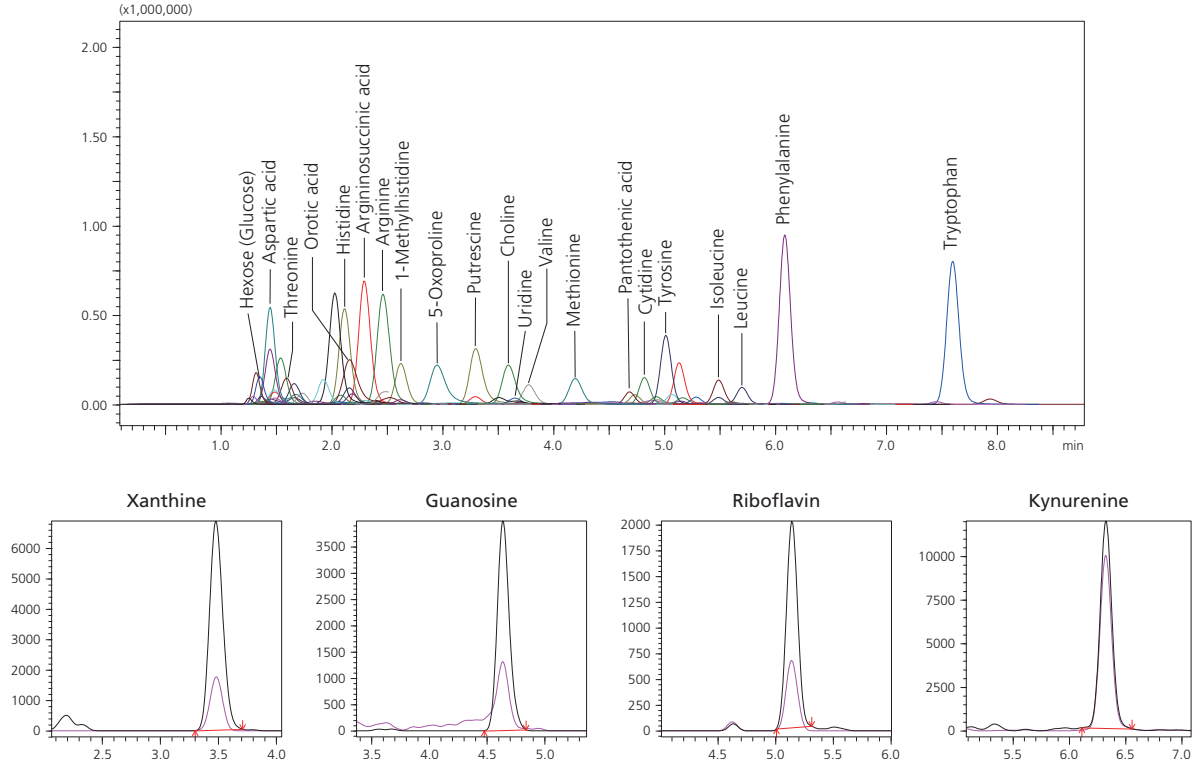
This Method Package enables the analysis of 125 compounds in under 20 minutes per sample. Performing analysis separately for each compound group such as amino acids and vitamins makes profiling of cell culture components very laborious, but with this method package a large number of culture medium components and secreted metabolites can be analyzed simultaneously.

Compared to the previous version, several metabolites derived from amino acids, nucleic acids and the TCA cycle have been added, allowing even more comprehensive profiling information to be gathered.

Optimized Method for Culture Medium Analysis

Pre-set analysis conditions make full use of triple quadrupole MS capabilities for analyzing trace components such as vitamins. On the other hand, analysis conditions are adjusted so that high-concentration components such as glucose or amino acids are not saturated. It is possible to measure a variety of culture medium components from the same vial.

Note: A dilution series must be created for accurate quantification.



Analysis of culture supernatant

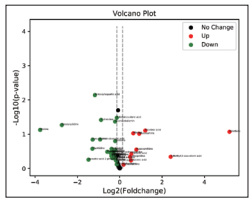
Ready-to-Use Method

Analysis can be started without the need for time-consuming preparations such as optimization of MS parameters for each compound or careful consideration of LC/MS/MS analysis conditions.

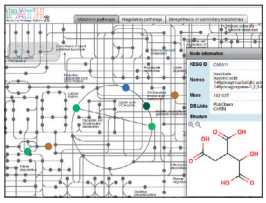
Excellent Data Analysis Functionality

Using the Multiomics Analysis Package, it is easy and straightforward to compare changes in compound quantities on a bar graph, display changes over time on a line chart, etc.

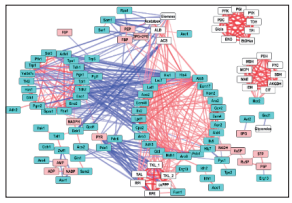
It also includes easy-to-implement functions for correlation analysis, volcano plots, and more, significantly reducing the time required for bottleneck processes such as data analysis and visualization. The whole workflow from measurement to data analysis becomes smoother and more efficient.



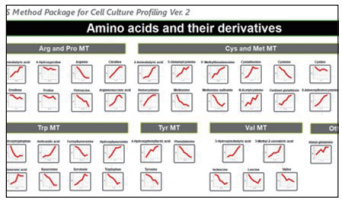
Volcano plot display



Visualization of compounds showing changes on the volcano plot



Visual representation of related compounds



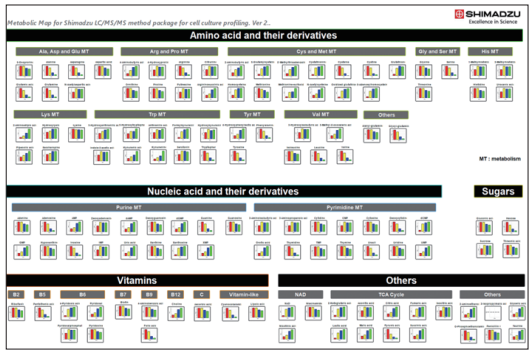
Display of changes over time

Data Analysis Example

Data obtained with the method package can be inserted on the included metabolic map. It is then simple to compare compound quantities on a bar graph or display changes over time on a line graph.

Time-series measurement data

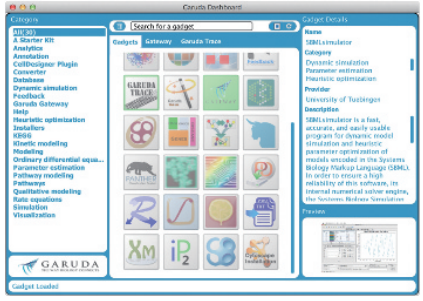
Select files



A blank map for Cell Culture Profiling Ver. 2 is included with the method package installer

Tools for Data Analysis

The data analysis software in this Method Package is 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/

POWERED BY GARUDA

Data Analysis Tools in the Method Package

Volcano Plot
A tool that combines a t-test (for statistically significant differences) and a fold analysis (e.g. twice or half the mean value) to visualize the differences between the two groups. The Volcano Plot gadget developed by Shimadzu is included in the package.

VANTED
Supports data analysis of biological processes through metabolic profiling and visualization of enzyme activity on metabolic maps. 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, integrate gene expression profiles with related data, etc. It is especially useful for analyzing networks and visualizing correlations.

List of Registered Compounds

Amino acids and their metabolites	Group
5-Oxoproline	Ala, Asp and Glu MT
Alanine	Ala, Asp and Glu MT
Asparagine	Ala, Asp and Glu MT
Aspartic acid	Ala, Asp and Glu MT
Glutamic acid	Ala, Asp and Glu MT
Glutamine	Ala, Asp and Glu MT
N-Acetylaspartic acid	Ala, Asp and Glu MT
4-Aminobutyric acid	Arg MT
4-Hydroxyproline	Arg MT
Arginine	Arg MT
Citrulline	Arg MT
Ornithine	Arg MT
Proline	Arg MT
Putrescine	Arg MT
Argininosuccinic acid	Arg MT
2-Aminobutyric acid	Cys and Met MT
5-Glutamylcysteine	Cys and Met MT
5'-Methylthioadenosine	Cys and Met MT
Cystathionine	Cys and Met MT
Cysteine	Cys and Met MT
Cystine	Cys and Met MT
Glutathione	Cys and Met MT
Homocysteine	Cys and Met MT
Methionine	Cys and Met MT
Methionine sulfoxide	Cys and Met MT
N-Acetylcysteine	Cys and Met MT
Oxidized glutathione	Cys and Met MT
S-Adenosylhomocysteine	Cys and Met MT
Glycine	Gly and Ser MT
Serine	Gly and Ser MT
Threonine	Gly and Ser MT
1-Methylhistidine	His MT
3-Methylhistidine	His MT
Histidine	His MT
Urocanic acid	His MT
2-Aminoadipic acid	Lys MT
Hydroxylysine	Lys MT
Lysine	Lys MT
Pipecolic acid	Lys MT
Saccharopine	Lys MT
3-Hydroxyanthranilic acid	Trp MT
5-Hydroxytryptophan	Trp MT
Anthranilic acid	Trp MT
Formylkynurenine	Trp MT
Hydroxykynurenine	Trp MT
Indole-3-acetic acid	Trp MT
Kynurenic acid	Trp MT

Amino acids and their metabolites	Group
Kynurenine	Trp MT
Serotonin	Trp MT
Tryptophan	Trp MT
4-Hydroxyphenyllactic acid	Tyr MT
Phenylalanine	Tyr MT
Tyrosine	Tyr MT
3-Hydroxyisobutyric acid	Val MT
3-Methyl-2-oxovaleric acid	Val MT
Isoleucine	Val MT
Leucine	Val MT
Valine	Val MT
Alanyl-glutamine	—
Glycyl-glutamine	—

Nucleic acids and their metabolites	Group
Adenine	Purine MT
Adenosine	Purine MT
Adenosine monophosphate	Purine MT
Deoxyadenosine	Purine MT
Deoxyadenosine monophosphate	Purine MT
Deoxyguanosine	Purine MT
Deoxyguanosine monophosphate	Purine MT
Guanine	Purine MT
Guanosine	Purine MT
Guanosine monophosphate	Purine MT
Hypoxanthine	Purine MT
Inosine	Purine MT
Inosine monophosphate	Purine MT
Uric acid	Purine MT
Xanthine	Purine MT
Xanthosine	Purine MT
Xanthosine monophosphate	purine MT
3-Aminoisobutyric acid	Pyrimidine MT
3-Aminopropanoic acid	Pyrimidine MT
Cytidine	Pyrimidine MT
Cytidine monophosphate	Pyrimidine MT
Cytosine	Pyrimidine MT
Deoxycytidine	Pyrimidine MT
Deoxycytidine monophosphate	Pyrimidine MT
Orotic acid	Pyrimidine MT
Thymidine	Pyrimidine MT
Thymidine monophosphate	Pyrimidine MT
Thymine	Pyrimidine MT
Uracil	Pyrimidine MT
Uridine	Pyrimidine MT
Uridine monophosphate	Pyrimidine MT

Sugars	Group
Gluconic acid	—
Hexose (Glucose)	—
Sucrose	—
Threonic acid	—

Vitamins	Group
Riboflavin	B2
Niacinamide	B3
Nicotinic acid	B3
Pantothenic acid	B5
4-Pyridoxic acid	B6
Pyridoxal	B6
Pyridoxalphosphate	B6
Pyridoxine	B6
Biotin	B7
4-Aminobenzoic acid	B9
Folic acid	B9
Choline	B12
Ascorbic acid	C
Cyanocobalamin	Vitamin-like
Lipoic acid	Vitamin-like

Others	Group
2-ketoglutaric acid	TCA Cycle
Acotinic acid	TCA Cycle
Citric acid	TCA Cycle
Fumaric acid	TCA Cycle
Isocitric acid	TCA Cycle
Lactic acid	TCA Cycle
Malic acid	TCA Cycle
Pyruvic acid	TCA Cycle
Succinic acid	TCA Cycle
Penicillin G	Antibiotics
2-Aminoethanol	—
Glyceric acid	—
NAD	—
O-Phosphoethanolamine	—
Taurine	—

Internal standard	Group
2-Isopropylmalic acid	—

*MT: metabolism

Cautions

1. LabSolutions LCMS Ver. 5.97 or later is required.
2. 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.

LabSolutions and LCMS are trademarks of Shimadzu Corporation.
GARUDA is a trademark of The Systems Biology Institute.

Shimadzu Corporation
www.shimadzu.com/an/

For Research Use Only. Not for use in diagnostic procedures.
This publication may contain references to products that are not available in your country. Please contact us to check the availability of these products in your country.
Company names, products/service names and logos used in this publication are trademarks and trade names of Shimadzu Corporation, its subsidiaries or its affiliates, whether or not they are used with trademark symbol "TM" or "®".
Third-party trademarks and trade names may be used in this publication to refer to either the entities or their products/services, whether or not they are used with trademark symbol "TM" or "®".
Shimadzu disclaims any proprietary interest in trademarks and trade names other than its own.

The contents of this publication are provided to you "as is" without warranty of any kind, and are subject to change without notice. Shimadzu does not assume any responsibility or liability for any damage, whether direct or indirect, relating to the use of this publication.

© Shimadzu Corporation, 2020
First Edition: February 2020 3655-02005-ODPIT