C146-E456C

SHIMADZU
Excellence in Science

Smart Metabolites Database for GC-MS(/MS) Analysis

Smart Metabolites Database Ver. 2

Supporting food development with newly added sugars and functional compounds

The Smart Metabolites Database™ is a GC-MS(/MS) database that contains the information needed for analyzing metabolic compounds. Ver. 2 contains an additional number of registered compounds, focusing on plant secondary metabolites, such as catechins and chlorogenic acids, that are garnering interest as functional compounds, for more expansive analysis of food samples. In total, the Smart Metabolites Database Ver. 2 enables simultaneous analysis of more than 600 compounds, making it a powerful tool for marker discovery in metabolomics analysis.
The database also offers dedicated methods for fatty acids, and sugars and provides total support for metabolic compound analysis.

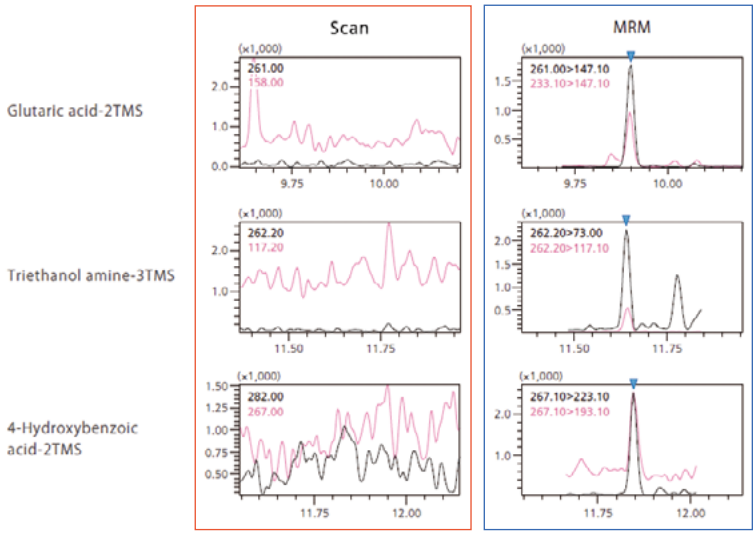
Number of Registered Compounds

	Derivatization Method	Analytical Method	Number of Registered Compounds
For Comprehensive Analysis			
Simultaneous analysis of metabolic compounds	TMS	SIM	627
		MRM	540
For Individual Compound Analysis			
Fatty acids	Methylation	SIM MRM	50
Sugars	Acetylation	SIM MRM	24

This database was developed through guidance from the Shimane University Faculty of Medicine, Kobe University School of Medicine, the Institute for Integrated Cell-Material Sciences, Kyoto University, Hyogo College of Medicine and Graduate School of Engineering, Osaka University. Part of this database was obtained as a result of development work related to the project for "Development of fundamental technologies for promoting industrial application of human stem cells and development of fundamental evaluation technologies for practical application of human stem cells" commissioned by Japan's New Energy and Industrial Technology Development Organization (NEDO).

Automated, Highly Sensitive Detection of Metabolic Compounds by MRM Measurement

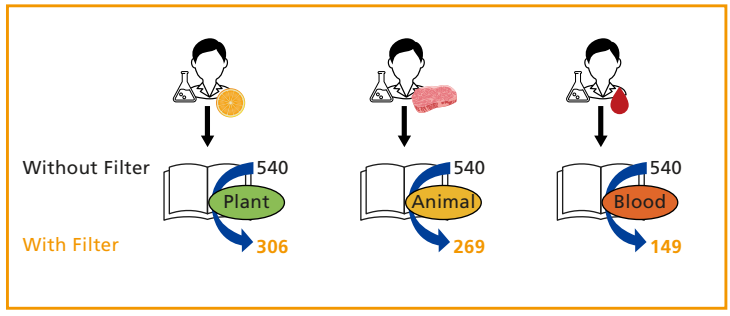
Metabolite analysis has conventionally been performed using scan methods; however, these methods often suffer from issues such as insufficient sensitivity to detect trace compounds, overlapping metabolites, and contaminants interfering with accurate results.
In this database, wide-target analysis using MRM can detect metabolic compounds with high sensitivity and selectivity, thus accurate results can be obtained even when analyzing for trace compounds. When combined with highly reliable metabolite identification based on retention indices, users can obtain highly accurate results in comparative analysis of foods and marker discovery.



Time and Labor Savings

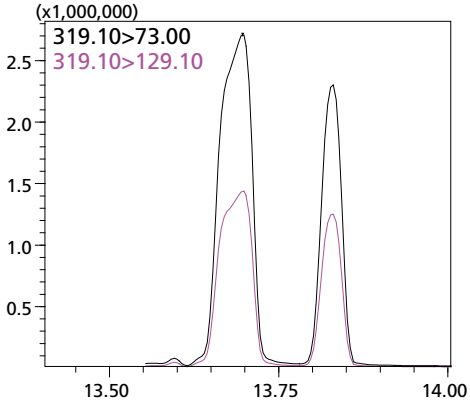
The Smart Metabolites Database includes more than 600 compounds and facilitates metabolite analysis across a wide variety of samples. Nevertheless, the greater the number of compounds analyzed, the more time needed for data analysis. To minimize this issue, the Smart Metabolites Database comes with a new filter function that allows users to select and analyze only those metabolic compounds likely to be detected in a given sample, thereby saving time and labor in the analysis process. This filter function can be turned on and off at user discretion.

Filter	No. of Compounds
All registered compounds (MRM)	540
Plant (food)	306
Animal (food)	269
Blood (plasma)	149
Urine	171
Cells	224



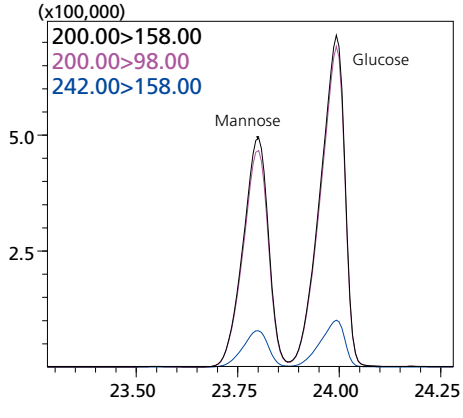
Offers Quantitative Sugar Analysis

The methoxime-TMS derivatization method is in common use, but produces multiple geometric isomers from reducing sugars and causes chain formation due to derivatization, making chromatographic separation of sugar isomers not possible.
A new sugar quantification method uses an optimized derivatization method to enable the selective detection of sugars. The database also contains compound information and calibration curve information needed to analyze 24 major sugars, allowing semi-quantitative results to be calculated for detected sugars.
The extraction procedure used on samples is identical to that used by simultaneous metabolite analysis, thus simultaneous metabolite analysis and quantitative sugar analysis can both be performed on the same processed sample.



Methoxime-TMS Method

Unable to separate mannose and glucose.
Two peaks are detected, each a mixture of mannose and glucose.



Sugar-Specific Method

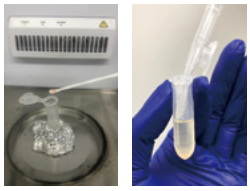
Able to selectively detect sugars

*Semi-quantitative results may vary significantly from true values depending on equipment conditions and sample preparation. Quantitative tests should be performed with standard samples if accurate quantitative results are required.

Total Support for Food Metabolomics Analysis

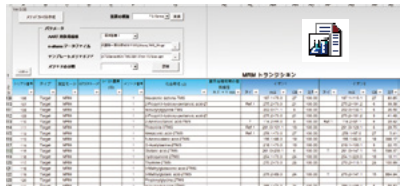
Shimadzu provides complete support for GC/MS food metabolomics analysis from sample preparation to multivariate analysis. The "Metabolomics Handbook" compiles practical information on food sample preparation, allowing even newcomers to food metabolomics to output results up to and including multivariate analysis.

Sample Preparation
(Metabolomics Handbook)



Explains sample preparation with easy-to-understand photographs. Suggests preparation methods appropriate for food type.

Method File Creation
(Smart Metabolites Database Ver. 2)



Predicts retention times of registered compounds based on retention times of *n*-alkanes and automatically creates analytical methods.

Analysis

Highly sensitive, widely targeted analysis using SIM/MRM.

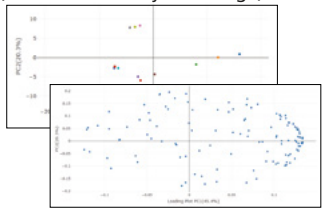
Multi-Sample Data Analysis (LabSolutions Insight™*)

List Output

Stress-free batch analysis of multi-sample data

Visualization on Metabolic Maps And Multivariate Analysis (Multi-omics Analysis Package)

Automatic visualization with templates



Output analysis results with minimal setup

* LabSolutions Insight and Multi-omics Analysis Package are not included in this product.

Product Contents

Database file (Excel®), method file, library file, batch file, damlp file for LabSolutions Insight

Compatible Instruments

GC-MS:	GCMS-QP2020, GCMS-QP2050, GCMS NX series
Autosamplers:	AOC™-30/20 series, AOC-6000 series
Excel®:	Microsoft® Excel® 2021 (32-bit or 64-bit version), 2019 (32-bit or 64-bit version)
Workstation:	GCMSsolution™ + LabSolutions Insight LabSolutions™ GCMS + LabSolutions Insight LabSolutions™ DB GCMS/LabSolutions CS + LabSolutions Insight DB/CS

Recommended Consumables

n-Alkanes:	C7-C33 : Qualitative Retention Time Index Standard (Restek 31080)
Analytical Column:	DB-5 30m x 0.25mm I.D. df=1.00 um (Agilent Cat No. 122-5033) BPX-5 30m x 0.25mm I.D. df=0.25 um (SGE Cat No. 054101) DB-5MS 30m x 0.25mm I.D. df=0.25 um (Agilent Cat No. 122-5532) SP2560 100m x 0.25mm I.D. df=0.20 um (Supelco Cat No. 24056)

Precautions

1. The accuracy of the information contained in the database and the usefulness of information obtained as a result of the use of this information is not guaranteed.
2. Be sure to test the qualitative and quantitative information obtained with this system using a standard sample for confirmation.
3. To reliably identify substances registered with this database, perform measurement using the system requirements of the method file included with the product.
4. This database is for research use only. Not for use in diagnostic procedures.

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