C146-E437

SHIMADZU
Excellence in Science

For LabSolutions LCMS

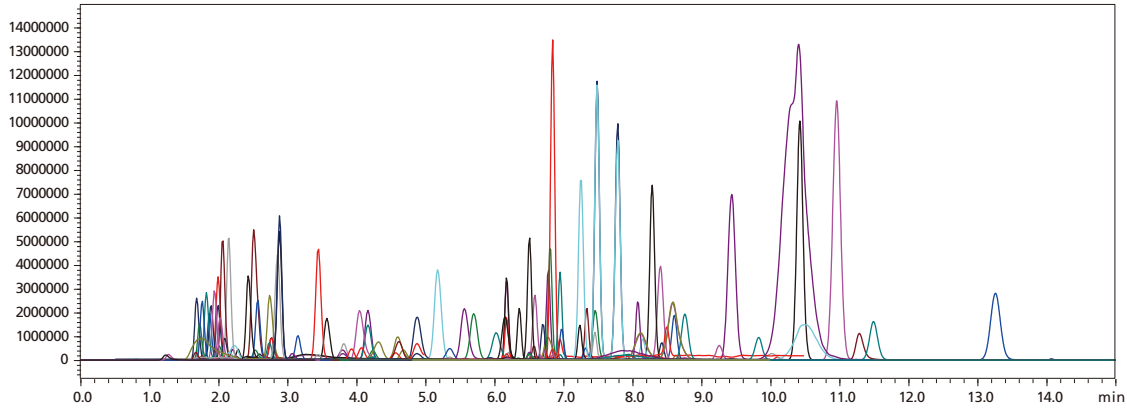
LC/MS/MS Method Package for Primary Metabolites Ver.3

Ready-to-use methods for 200 compounds

This Method Package enables efficient, simultaneous analysis of a large number of compounds. Optimized LC separation conditions and MS parameters reduce the time and effort expended on method development.

Choice of optimized analysis conditions

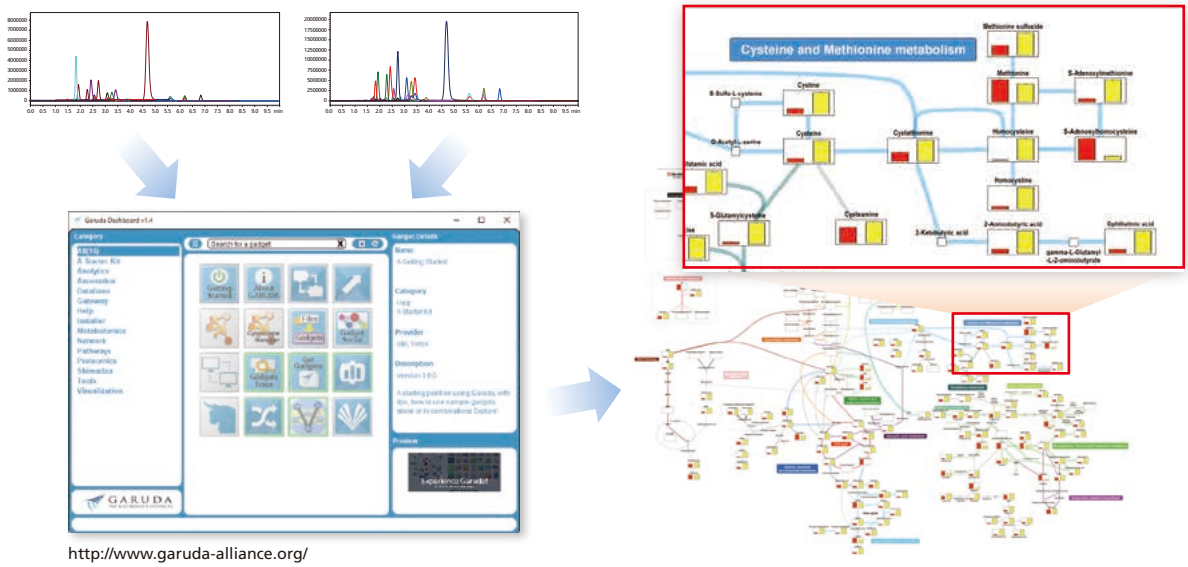
Choose between two method types to suit your analysis aims and equipment. The ion-pair reagent method (112 compounds) is particularly useful for the analysis of sugar phosphates, while the non-ion-pair reagent method (141 compounds), effective in the research of high-value-added substances, does not require ion-pair reagents and in this version has been expanded to include compounds involved in the mevalonate and shikimic acid pathways.



Overlaid MRM chromatograms for simultaneous analysis of a mixture of 141 standards with the non-ion-pair reagent method

Visualization of metabolic changes

With the included Multi-omics Data Analysis Package, quantitative data can be visualized easily on a metabolic map.



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

Visualization of simultaneous analysis results from the PFPP column method, created with the Multi-omics Data Analysis Package

Compatible with the Nexera™ series and the LCMS-8060NX

All methods are compatible with both the Nexera series and the LCMS-8045/8050/8060 (NX), covering a wide range of analysis needs.

A total solution from pretreatment to analysis

This Method Package includes protocols for preparing biological tissue extracts, enabling stable analysis with proven pretreatment techniques and reducing the labor and expense involved in method development.

Index of compounds

List of compounds for the ion-pair reagent method

Glycolytic system	2,3-Bisphosphoglyceric acid 3-Phosphoglyceric acid (2-Phosphoglyceric acid) Dihydroxyacetone phosphate Fructose 1,6-bisphosphate Glucose 1-phosphate Glucose 6-phosphate Glycerol 3-phosphate Phosphoenolpyruvic acid Pyruvic acid
Pentose-phosphate pathway	Fructose 6-phosphate Glyceraldehyde 3-phosphate 6-Phosphogluconic acid Erythrose 4-phosphate Ribose 1-phosphate Ribose 5-phosphate Ribulose 5-phosphate Sedoheptulose 7-phosphate
Sugar phosphate	Fructose 1-phosphate Mannose 6-phosphate Phosphoribosyl pyrophosphate Ribulose 1,5-bisphosphate
TCA cycle	Acetyl coenzyme A 2-Ketoglutaric acid Succinyl coenzyme A
Amino acids	2-Aminobutyric acid 4-Aminobutyric acid Alanine Arginine Asparagine Aspartic acid Cysteine Glutamic acid Glutamine Glycine Histidine 4-Hydroxyproline Isoleucine Leucine Lysine Methionine Phenylalanine Proline Serine Threonine Tryptophan Tyrosine Valine
Co-enzyme	3-Hydroxybutyryl coenzyme A Butyryl coenzyme A Coenzyme A Crotonyl coenzyme A FAD FMN Malonyl coenzyme A Methylmalonyl coenzyme A NAD NADH NADP NADPH Nicotinic acid Pyrroloquinoline quinone
Non-mevalonic acid pathway	HMBPP IPP_DMAPP MEP
Shikimic acid pathway	Shikimic acid Shikimic acid 3-phosphate
Organic acids	2-Isopropylmalic acid 3-Hydroxyphenylacetic acid 4-Hydroxyphenyl pyruvic acid Citramalic acid Glyceric acid Glycerol 2-phosphate Glycerol 3-phosphate Glycolic acid Indole 3-acetic acid Pantothenic acid
Nucleosides and Nucleotides	Adenine Adenosine Adenosine 3',5'-cyclic monophosphate Adenosine diphosphate Adenosine monophosphate Adenosine triphosphate AICAR Cytidine Cytidine diphosphate Cytidine monophosphate Cytidine triphosphate Guanine Guanosine Guanosine 3',5'-cyclic monophosphate Guanosine diphosphate Guanosine monophosphate Guanosine triphosphate Inosine Inosine monophosphate Orotic acid Thymidine Thymidine diphosphate Thymidine monophosphate Thymidine triphosphate Thymine Uridine Uridine diphosphate Uridine monophosphate Uridine triphosphate Xanthosine monophosphate
Nucleotide sugar	ADP-glucose UDP-glucose
Purine derivative	Hypoxanthine Uric acid Xanthine
Internal STDs	2-Morpholinoethanesulfonic acid Methionine sulfone

List of compounds for the non-ion-pair reagent method

Glycolytic system	Lactic acid
	Pyruvic acid
TCA cycle	2-Ketoglutaric acid
	Aconitic acid
	Citric acid
	Fumaric acid
	Isocitric acid
	Malic acid
	Succinic acid
Urea cycle	Argininosuccinic acid
	Ornithine
	Citrulline
Amino acids	4-Hydroxyproline
	Alanine
	Anthranilic acid
	Arginine
	Asparagine
	Aspartic acid
	Asymmetric dimethylarginine
	Cystine
	Dimethylglycine
	Glutamic acid
	Glutamine
	Glycine
	Histidine
	Homocystine
	Isoleucine
	Leucine
	Lysine
	Methionine sulfoxide
	Phenylalanine
	Proline
	Serine
	Symmetric dimethylarginine
	Threonine
	Tryptophan
	Valine
Methylation and Transsulfuration cycle	Cystathionine
	Cysteine
	Homocysteine
	Methionine
	5-Glutamylcysteine
	Glutathione
	Oxidized glutathione
	S-Adenosylhomocysteine
	S-Adenosylmethionine
Shikimic acid pathway	3-Dehydroquinic acid
	3-Dehydroshikimic acid
	Chorismic acid
	Shikimic acid
	Shikimic acid 3-phosphate
Organic acids	2-Aminobutyric acid
	4-Aminobenzoic acid
	4-Aminobutyric acid
	Caffeic acid
	Cholic acid
	Creatine
	Ferulic acid
	Glycolic acid
	Glyoxylic acid
	Ophthalmic acid
	Orotic acid
	p-Coumaric acid
	Phenyllactic acid
	Phenylpyruvic acid
	Taurocholic acid
	Urocanic acid
	Vanillic acid
Catecholamine	Dopamine
	Epinephrine
	Norepinephrine
	Serotonin
Vitamin B	Folic acid
	Pantothenic acid
	PLP
Nucleosides and Nucleotides	Adenine
	Adenosine
	Adenosine 3',5'-cyclic monophosphate
	Adenosine monophosphate
	Adenylsuccinic acid
	AICAR
	Cytidine
	Cytidine 3',5'-cyclic monophosphate
	Cytidine monophosphate
	Cytosine
	Guanine
	Guanosine
	Guanosine 3',5'-cyclic monophosphate
	Guanosine monophosphate
	Inosine
	Thymidine
	Thymidine monophosphate
	Thymine
	Tyrosine
	Uracil
	Uridine
Purine derivative	Allantoin
	Hypoxanthine
	Uric acid
	Xanthine
Co-enzyme	FAD
	FMN
	NAD
	Niacinamide
	Nicotinic acid
Non-mevalonic acid pathway	DOXP
	MEP
Mevalonic acid pathway	Mevalonic acid
	MVA-P
Alkaloid	Higenamine
	Reticuline
	THP
Others	4-Aminophenylalanine
	4-Aminophenylpyruvic acid
	4-Hydroxybenzoic acid
	Acetylcarnitine
	Acetylcholine
	Carnitine
	Carnosine
	Catechol
	Choline
	Citicoline
	Creatinine
	Cysteamine
	Dihydroxyphenylacetaldehyde
	Dihydroxyphenylacetic acid
	Dopa
	Ergothioneine
	Histamine
	Histidinol
	Hydroxytyrosol
	Indole
	Kynurenine
	Methyl-DOPA
	Protocatechuic acid
	Protocatechuic aldehyde
	Resveratrol
	Salicylic acid
	Sinapic acid
	Tyramine
	Vanillin
Internal STDs	2-Morpholinoethanesulfonic acid
	Methionine sulfone

* With this method package, choose between the ion-pair reagent method (112 compounds) or the PFPP column method (141 compounds) depending on your equipment and analysis aims.

Precautions

LabSolutions LCMS Ver.5.99 SP2 or later is required.
This method package is for research use only.

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