SHIMADZU
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C146-E401

LabSolutions™ LCMS for LCMS-9030

Exact Mass Database for Endogenous Metabolites

Ready-to-use methods for metabolomics

The physical properties of target compounds in metabolomics can vary greatly. An analysis method tailored to the target compounds is therefore needed for comprehensive measurements of metabolites.

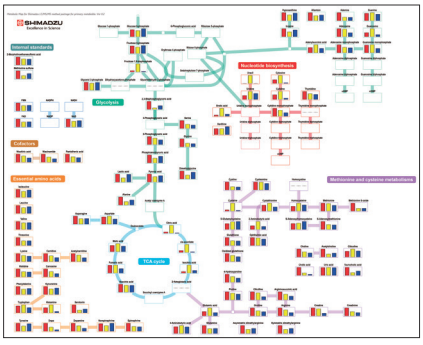
This database contains multiple ready-to-use methods for comprehensive analysis of metabolites with different properties. Pretreatment examples are also included for various metabolites and samples. The user can begin a metabolomics analysis without time-consuming evaluation of LC or MS conditions.

Information for 470 compounds

This database is based on the successful LC/MS/MS Method Packages for Primary Metabolites, Cell Culture Profiling, Lipid Mediators, Short Chain Fatty Acids, and Bile Acids, and provides a comprehensive list of 470 metabolites (including internal standards) with retention times and exact mass information.

Method name	No. of registered compounds
Primary metabolites	99
Cell culture profiling	96
Lipid mediators	214
Short chain fatty acids	23
Bile acids	38

The database is compatible with the Multi-omics Analysis Package (sold separately). Processing the analysis results with the Multi-omics Analysis Package allows metabolic mapping, network analysis and projection on the metabolic map to be carried out easily.



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

List of registered compounds

Category	Compound name	P.M.	C.C.	L.M.	S.C.	B.A
Amino acids	4-Hydroxyproline	○				
	5-Oxoproline		○			
	Acetylcarnitine	○				
	Alanine	○	○			
	Alanyl-glutamine		○			
	Arginine	○	○			
	Asparagine	○	○			
	Aspartic acid	○	○			
	Asymmetric dimethylarginine	○				
	Citrulline	○	○			
	Cystathionine	○	○			
	Cysteine	○	○			
	Cystine	○	○			
	Cytosine	○				
	Dimethylglycine	○				
	Glutamic acid	○	○			
	Glutamine	○	○			
	Glycine	○	○			
	Glycyl-glutamine		○			
	Histidine	○	○			
	Homocysteine	○				
	Homocystine	○				
	Isoleucine	○	○			
	Leucine	○	○			
	Lysine	○	○			

Category	Compound name	P.M.	C.C.	L.M.	S.C.	B.A
Amino acids	Methionine	○	○			
	Methionine sulfoxide	○	○			
	N-Acetylaspartic acid		○			
	N-Acetylcysteine		○			
	Ornithine	○	○			
	Phenylalanine	○	○			
	Pipecolic acid		○			
	Proline	○	○			
	Serine	○	○			
	Symmetric dimethylarginine	○				
	Threonine	○	○			
	Tryptophan	○	○			
	Tyrosine	○	○			
	Valine	○	○			
Organic acids	2-Aminobutyric acid	○	○			
	2-Ethylbutyric acid				○	
	2-Hydroxyglutaric acid				○	
	2-Isopropylmalic acid		○			
	2-Ketoglutaric acid	○			○	
	2-Ketoisovaleric acid		○			
	2-Oxobutyric acid				○	
	4-Aminobutyric acid	○	○			
	Acetic acid				○	
	Aconitic acid	○				
	Adenylsuccinic acid	○				

Category	Compound name	P.M.	C.C.	L.M.	S.C.	B.A
Organic acids	Argininosuccinic acid	○				
	beta-Hydroxybutyric acid				○	
	Butyric acid				○	
	Citric acid	○	○		○	
	Creatine	○				
	Fumaric acid	○	○		○	
	Gluconic acid		○			
	Glycolic acid				○	
	Glyoxylic acid				○	
	Isobutyric acid				○	
	Isocitric acid	○	○		○	
	Isovaleric acid				○	
	Lactic acid	○	○		○	
	Maleic acid				○	
	Malic acid	○	○		○	
	Malonic acid				○	
	Methionine sulfone	○				
	Nicotinic acid	○	○			
	Ophthalmic acid	○				
	Orotic acid	○				
	Oxaloacetic acid				○	
	Pantothenic acid	○	○			
	Propionic acid				○	
	Pyruvic acid	○	○		○	
	Succinic acid	○	○		○	
	Threonic acid		○			
	Uric acid	○	○			
	Valeric acid				○	
Bile acids	12-keto-Deoxycholic acid					○
	7-keto-Deoxycholic acid					○
	7-keto-Lithocholic acid					○
	allo-Chenodeoxycholic acid					○
	allo-Lithocholic acid					○
	Chenodeoxycholic acid					○
	Cholic acid	○				○
	Deoxycholic acid					○
	Glycochenodeoxycholic acid					○
	Glycocholic acid					○
	Glycodeoxycholic acid					○
	Glycohyodeoxycholic acid					○
	Glycolithocholic acid					○
	Glycoursodeoxycholic acid					○
	Hyodeoxycholic acid					○
	Lithocholic acid					○
	Tauro-a-muricholic acid					○
	Tauro-b-muricholic acid					○
	Taurochenodeoxycholic acid					○
	Taurocholic acid	○				○
	Taurodeoxycholic acid					○
	Taurohyodeoxycholic acid					○
	Taurolithocholic acid					○
	Tauroursodeoxycholic acid					○
	Ursodeoxycholic acid					○
	α-Muricholic acid					○
	β-Muricholic acid					○
	ω-Muricholic acid					○
Nucleic-acid-related	Adenine	○	○			
	Adenosine	○	○			
	Adenosine 3',5'-cyclic monophosphate	○				
	Adenosine monophosphate	○	○			
	Citicoline	○				
	Cytidine	○	○			
	Cytidine 3',5'-cyclic monophosphate	○				
	Cytidine monophosphate	○	○			
	Deoxycytidine		○			
	Guanine	○	○			
	Guanosine	○	○			
	Guanosine 3',5'-cyclic monophosphate	○				
	Guanosine monophosphate	○	○			
	Inosine	○	○			
	Thymidine	○	○			
	Thymidine monophosphate	○				
	Thymine	○	○			
	Uracil	○	○			
	Uridine	○	○			

Category	Compound name	P.M.	C.C.	L.M.	S.C.	B.A
Nucleic-acid-related	Xanthine	○	○			
	Xanthosine		○			
Vitamins	4-Aminobenzoic acid		○			
	4-Hydroxyphenyllactic acid	○	○			
	Ascorbic acid		○			
	Ascorbic acid 2-phosphate		○			
	Biotin		○			
	Cyanocobalamin		○			
	Ergocalciferol		○			
	Folic acid		○			
	Folinic acid		○			
	Lipoic acid		○			
	Niacinamide	○	○			
	Pyridoxal		○			
	Pyridoxine		○			
	Riboflavin		○			
	Tocopherol acetate		○			
Lipid mediators	11(S)-HETE			○		
	11-trans LTC4			○		
	11-trans LTD4			○		
	11-trans LTE4			○		
	11β-Prostaglandin E2			○		
	11β-Prostaglandin F2α			○		
	12(S)-HETE			○		
	12(S)-HHTrE			○		
	12-oxo LTB4			○		
	15(S)-HETE			○		
	15(S)-HpETE			○		
	15-keto Prostaglandin E2			○		
	15-keto Prostaglandin F1α			○		
	15-keto Prostaglandin F2α			○		
	15-OxoETE			○		
	18-carboxy dinor LTB4			○		
	19(S)-HETE			○		
	20-carboxy arachidonic acid			○		
	20-carboxy leukotriene B4			○		
	20-HETE			○		
	20-hydroxy leukotriene B4			○		
	20-hydroxy Prostaglandin E2			○		
	20-hydroxy Prostaglandin F2α			○		
	5(S),14(R)-LXB4			○		
	5(S)-HEPE			○		
	5(S)-HETE			○		
	5(S)-HETrE			○		
	5(S)-HpEPE			○		
	5(S)-HpETE			○		
	5-OxoETE			○		
	6-keto Prostaglandin E1			○		
	6-keto-Prostaglandin F1α			○		
	6-trans LTB4			○		
	7(R)-Maresin 1			○		
	8(S),15(S)-DiHETE			○		
	8(S)-HEPE			○		
	8(S)-HETE			○		
	8(S)-HETrE			○		
	8-iso Prostaglandin A1			○		
	8-iso Prostaglandin A2			○		
	8-iso Prostaglandin E1			○		
	8-iso Prostaglandin E2			○		
	9(S)-HEPE			○		
	Arachidonic Acid (AA)			○		
	Arachidonoyl ethanolamide			○		
	Azelaoyl PAF			○		
	Docosahexaenoic Acid (DHA)			○		
	Eicosapentaenoic Acid (EPA)			○		
	iPF2α-IV			○		
	Leukotriene B3			○		
	Leukotriene B4			○		
	Leukotriene B5			○		
	Leukotriene C4			○		
	Leukotriene D4			○		
	Leukotriene E4			○		
	Leukotriene F4			○		
	Lipoxin A5			○		
	LTB4 ethanolamide			○		

P.M. = Primary metabolites method, C.C. = Cell culture profiling method, L.M. = Lipid mediators methods, S.C. = Short chain fatty acids method, B.A. = Bile acids method
This database contains retention times and exact mass information for 470 metabolites including the above metabolites and internal standards
* Compatible devices: LCMS-9030

List of registered compounds

Category	Compound name	P.M.	C.C.	L.M.	S.C.	B.A
Lipid mediators	N-acetyl LTE4			○		
	OEA (oleoyl ethanolamide)			○		
	PAF C-16			○		
	Prostaglandin A1			○		
	Prostaglandin A2			○		
	Prostaglandin D1			○		
	Prostaglandin D2			○		
	Prostaglandin D3			○		
	Prostaglandin E1			○		
	Prostaglandin E2			○		
	Prostaglandin E3			○		
	Prostaglandin F1α			○		
	Prostaglandin F2α			○		
	Prostaglandin F3α			○		
	Prostaglandin J2			○		
	Prostaglandin K2			○		
	Prostagrandin D2 Ethanolamide			○		
	Prostagrandin E1 ethanolamide			○		
	Prostagrandin E2 Ethanolamide			○		
	Prostagrandin F2α Ethanolamide			○		
	Resolvin D1			○		
	Resolvin D2			○		
	Resolvin D3			○		
	Resolvin D4			○		
	Resolvin D5			○		
	Resolvin E1			○		
	tetranor-12(S)-HETE			○		
	tetranor-PGAM			○		
	tetranor-PGDM			○		
	tetranor-PGEM			○		
	tetranor-PGFM			○		
	tetranor-PGJM			○		
	Thromboxane B1			○		
	Thromboxane B2			○		

Category	Compound name	P.M.	C.C.	L.M.	S.C.	B.A
Others	2-Aminoethanol		○			
	2-Morpholinoethanesulfonic acid	○				
	3-Methyl-2-oxovaleric acid		○			
	5-Glutamylcysteine	○	○			
	Acetylcholine	○				
	Allantoin	○				
	Carnitine	○				
	Carnosine	○				
	Choline	○	○			
	Creatinine	○				
	Cysteamine	○				
	Dopa	○				
	Dopamine	○				
	Epinephrine	○				
	Ethylenediamine		○			
	FAD	○				
	FMN	○				
	Glucosamine		○			
	Glutathione	○	○			
	Glyceric acid		○			
	Hexose (Glucose)		○			
	Histamine	○	○			
	Hypoxanthine	○	○			
	Kynurenine	○	○			
	NAD	○				
	Norepinephrine	○				
	O-Phosphoethanolamine		○			
	Oxidized glutathione	○	○			
	Penicillin G		○			
	Putrescine		○			
	S-Adenosylhomocysteine	○				
	S-Adenosylmethionine	○				
	Serotonin	○				
	Sucrose		○			

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Precautions

1. LabSolutions LCMS Ver. 5.97 or later is required
2. This method package is for research use only. Not for use in diagnostic procedures.

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