

MxQuant kit

List of metabolites

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MxQuant kit – List of metabolites

Explore the small molecules shaping core metabolism

The MxQuant kit delivers a broad spectrum of small molecules for quantitative metabolomics deciphering microbiome-host interactions and core metabolism. Powered by biocrates' standardized, quality-controlled, and reproducible metabolomics technology, the ready-to-use kit covers 327 metabolites across 24 biochemical classes.

Analyte class (number of metabolites)		Analytical method
Small molecules (327)	Alkaloids (2)	LC-MS/MS
	Amine oxides (1)	
	Amino acids (20)	
	Amino acid-related (77)	
	Bile acids (24)	
	Biogenic amines (10)	
	Carboxylic acids (8)	
	Catechols (3)	
	Cresols (2)	
	Dicarboxylic acids (25)	
	Fatty acids (39)	
	Hormones and related (5)	
	Indoles and derivatives (18)	
	Nucleobases (5)	
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	Nucleotides (2)	
	Organic acids (16)	
	Phenolic acids (22)	
	Phenoxy compounds (2)	
	Polyamines (7)	
	Pyridinecarboxylic acids (6)	
	Sugars (7)	
	Tricarboxylic acids (3)	
	Vitamins and cofactors (9)	

Alkaloids (2)			
Nicotine	Nicotine	Trigonelline	Trigonelline

Amine oxides (1)			
TMAO	Trimethylamine N-oxide		

Amino acids (20)			
Ala	Alanine	Leu	Leucine
Arg	Arginine	Lys	Lysine
Asn	Asparagine	Met	Methionine
Asp	Aspartic acid	Phe	Phenylalanine
Cys	Cysteine	Pro	Proline
Gln	Glutamine	Ser	Serine
Glu	Glutamic acid	Thr	Threonine
Gly	Glycine	Trp	Tryptophan
His	Histidine	Tyr	Tyrosine
Ile	Isoleucine	Val	Valine

Amino acid-related (77)			
1-Met-His	1-Methylhistidine	Hypotaurine	Hypotaurine
3-Met-2-oxovaleric acid	3-Methyl-2-oxovaleric acid	Imidazole-propionic acid	Imidazolepropionic acid
3-Met-His	3-Methylhistidine	Kynurenine	Kynurenine
3-OH-Anthranilic acid	3-Hydroxyanthranilic acid	Met-SO	Methionine sulfoxide
3-OH-Kynurenine	3-Hydroxykynurenine	N2-Ac-Lys	N2-Acetyllysine
4-Guanidino-butanoic acid	4-Guanidinobutanoic acid	N6-Ac-Lys	N6-Acetyllysine
4-Met-2-oxovaleric acid	2-Oxoisocaproic acid	N-Ac-Ala	N-Acetylalanine
5-Amino-4-oxovaleric acid	5-Amino-4-oxovaleric acid	N-Ac-Arg	N-Acetylarginine
5-AVA	5-Aminovaleric acid	N-Ac-Asn	N-Acetylaspargine
5-OH-Trp	5-Hydroxytryptophan	N-Ac-Asp	N-Acetylaspartic acid
5-Oxo-Pro	5-Oxoproline	N-Ac-Gln	N-Acetylglutamine
AABA	α -Aminobutyric acid	N-Ac-Glu	N-Acetylglutamic acid
Ac-Orn	Acetylornithine	N-Ac-Gly	N-Acetyl glycine

Amino acid-related (77) continued			
ADMA	Asymmetric dimethylarginine	N-Ac-His	N-Acetylhistidine
Agmatine	Agmatine	N-Ac-Ile	N-Acetylisoleucine
α -Ketoiso-valeric acid	α -Ketoisovaleric acid	N-Ac-Leu	N-Acetylleucine
alpha-AAA	α -Aminoadipic acid	N-Ac-Met	N-Acetylmethionine
Anserine	Anserine	N-Ac-Phe	N-Acetylphenylalanine
Anthranilic - acid	Anthranilic acid	N-Ac-Pro	N-Acetylproline
Arginino-Suc	Argininosuccinic acid	N-Ac-Ser	N-Acetylserine
BABA	β -Aminobutyric acid	N-Ac-Trp	N-Acetyltryptophan
BAIBA	3-Aminoisobutyric acid	N-Ac-Tyr	N-Acetyltyrosine
Betaine	Betaine	N-Ac-Val	N-Acetylvaline
c4-OH-Pro	<i>cis</i> -4-Hydroxyproline	Nitro-Tyr	Nitrotyrosine
Carbamoyl-PO4	Carbamoylphosphate	N-Met-Asp	N-Methylaspartic acid
Carnosine	Carnosine	N-Nitroso-Pro	N-Nitrosoproline
Cinnamoyl-Gly	Cinnamoylglycine	Orn	Ornithine
Cit	Citrulline	PAG	Phenylacetylglutamine
Creatine	Creatine	PheAlaBetaine	Phenylalanine betaine
Creatinine	Creatinine	Phenylacetyl-glutamine	Phenylacetylglutamine
Cystine	Cystine	ProBetaine	Proline betaine
DMG	Dimethylglycine	Sarcosine	Sarcosine
DOPA	Dihydroxyphenylalanine	SDMA	Symmetric dimethylarginine
Furoyl-Gly	Furoylglycine	t4-OH-Pro	<i>trans</i> -4-Hydroxyproline
Guanidino-acetic acid	Guanidinoacetic acid	Taurine	Taurine
HArg	Homoarginine	TrpBetaine	Tryptophan betaine
HCit	Homocitrulline	Tryptamine	Tryptamine
HCys	Homocysteine	Tyramine	Tyramine
HSer	Homoserine		

Bile acids (24)			
12-KetoDCA	12-Ketodeoxycholic acid	IsoLCA	Isolithocholic acid
3-EpiDCA	3-Epideoxycholic acid	IsoUDCA	Isoursodeoxycholic acid
7-KetoDCA	7-Ketodeoxycholic acid	LCA	Lithocholic acid
CA	Cholic acid	NorDCA	Nordeoxycholic acid
CDCA	Chenodeoxycholic acid	TCA	Taurocholic acid
DCA	Deoxycholic acid	TCDC	Taurochenodeoxycholic acid
GCA	Glycocholic acid	TDCA	Taurodeoxycholic acid
GCDCA	Glycochenodeoxycholic acid	THDCA	Taurohyodeoxycholic acid

Bile acids (24) continued

GDCA	Glycodeoxycholic acid	TLCA	Taurolithocholic acid
GLCA	Glycolithocholic acid	TMCA	Tauromuricholic acids
GLCAS	Glycolithocholic acid sulfate	TUDCA	Tauroursodeoxycholic acid
GUDCA	Glycoursodeoxycholic acid	UDCA	Ursodeoxycholic acid

Biogenic amines (10)

beta-Ala	β -Alanine	Putrescine	Putrescine
GABA	γ -Aminobutyric acid	Serotonin	Serotonin
Dopamine	Dopamine	Spermidine	Spermidine
Histamine	Histamine	Spermine	Spermine
PEA	Phenylethylamine	Urea	Urea

Carboxylic acids (8)

2-OH-Butyric acid	2-Hydroxybutyric acid	HipAcid	Hippuric acid
3-OH-Butyric acid	3-Hydroxybutyric acid	Lac	Lactic acid
Glycolic acid	Glycolic acid	Mevalonic acid	Mevalonic acid
Glyoxylic acid	Glyoxylic acid	Pyruvic acid	Pyruvic acid

Catechols (3)

3,4-DiOH-Benzaldehyde	3,4-Dihydroxybenzaldehyde	Norepinephrine	Norepinephrine
Epinephrine	Epinephrine		

Cresols (2)

<i>p</i> -Cresol glucuronide	<i>p</i> -Cresol glucuronide	<i>p</i> -Cresol-SO ₄	<i>p</i> -Cresol sulfate
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Dicarboxylic acids (25)

2-OH-Glutaric acid	2-Hydroxyglutaric acid	Fumaric acid	Fumaric acid
3-HMGA	3-Hydroxymethylglutaric acid	Glutaric acid	Glutaric acid
3-Met-adipic acid	3-Methyladipic acid	Itaconic acid	Itaconic acid

Dicarboxylic acids (25) continued			
3-Met-glutaric acid	3-Methylglutaric acid	Maleic acid	Maleic acid
3-OH-Glutaric acid	3-Hydroxyglutaric acid	Malic acid	Malic acid
3-OH-Sebacic acid	3-Hydroxysebacic acid	Malonic acid	Malonic acid
Adipic acid	Adipic acid	Methylmalonic acid	Methylmalonic acid
α -Ketoglutaric acid	α -Ketoglutaric acid	Oxalic acid	Oxalic acid
Citramalic acid	Citramalic acid	Oxaloacetic acid	Oxaloacetic acid
DiCA 12:0	Dodecanedioic acid	Suberic acid	Suberic acid
DiCA 14:0	Tetradecanedioic acid	Suc	Succinic acid
E-3-Met-glutaconic acid	E-3-Methylglutaconic acid	Z-3-Met-glutaconic acid	Z-3-Methylglutaconic acid
Ethylmalonic acid	Ethylmalonic acid		

Fatty acids (39)			
FA 2:0	Acetic acid	FA 16:1	Palmitoleic acid
FA 3:0	Propanoic acid	FA 18:0	Stearic acid
FA 3:0-2M	Isobutyric acid	FA 18:1	Oleic acid
FA 4:0	Butyric acid	FA 18:2	Linoleic acid
FA 4:0-2M	2-Methylbutyric acid	FA 18:3	Octadecatrienoic acid
FA 4:0-3M	Isovaleric acid	FA 20:0	Arachidic acid
FA 5:0	Valeric acid	FA 20:1n-9	Gondoic acid
FA 5:0-3M	3-Methylvaleric acid	FA 20:2	Eicosadienoic acid
FA 5:0-4M	Isocaproic acid	FA 20:3n-6	Dihomo- γ -linolenic acid (ω 6)
FA 6:0	Caproic acid	FA 20:3n-9	Mead acid
FA 7:0	Heptanoic acid	FA 20:4n-6 (AA)	Arachidonic acid (AA; ω 6)
FA 8:0	Caprylic acid	FA 20:5n-3 (EPA)	Eicosapentaenoic acid (EPA; ω 3)
FA 9:0	Nonanoic acid	FA 22:0	Behenic acid
FA 10:0	Capric acid	FA 22:4n-6	Docosatetraenoic acid (ω 6)
FA 11:0	Undecanoic acid	FA 22:5n-3 (DPA)	Docosapentaenoic acid (DPA, ω 3)
FA 12:0	Lauric acid	FA 22:6n-3 (DHA)	Docosahexaenoic acid (DHA; ω 3)
FA 14:0	Myristic acid	FA 24:0	Lignoceric acid

Fatty acids (39) continued			
FA 14:1n-5	Myristoleic acid	FA 24:1n-9	Nervonic acid
FA 15:0	Pentadecanoic acid	FA 24:4n-6	Tetracosatetraenoic acid (ω6)
FA 16:0	Palmitic acid		

Hormones and related (5)			
Cortisol	Cortisol	T3	3,3',5-Triiodothyronine (T3)
Cortisone	Cortisone	T4	Thyroxine (T4)
DHEAS	Dehydroepiandrosterone sulfate		

Indoles and derivatives (18)			
3-IAA	3-Indoleacetic acid	Indoleacrylic acid	Indoleacrylic acid
3-IPA	3-Indolepropionic acid	Indolealdehyde	Indolealdehyde
5-HIAA	5-Hydroxyindoleacetic acid	Indole-Lac	Indolelactic acid
IAG	Indolylacryloylglycine	Indolepyruvic acid	Indolepyruvic acid
Indole-3-acetamide	Indole-3-acetamide	Indoxyl glucuronide	Indoxyl glucuronide
Indole-3-carboxylic acid	Indole-3-carboxylic acid	Ind-SO4	Indoxyl sulfate
Indole-3-ethanol	Indole-3-ethanol	Melatonin	Melatonin
Indole-3-methanol	Indole-3-methanol	Met-IAA	Methylindole-3-acetic acid
Indoleacet-aldehyde	Indoleacetaldehyde	Met-IPA	Methylindole-3-propionic acid

Nucleobases (5)			
Adenine	Adenine	Thymine	Thymine
Cytosine	Cytosine	Uracil	Uracil
Guanine	Guanine		

Nucleobase-related (14)			
Adenosine	Adenosine	Inosine	Inosine
AHCys	S-Adenosylhomocysteine	N-Ac-Cytidine	N4-Acetylcytidine
Cytidine	Cytidine	Orotic acid	Orotic acid

Nucleobase-related (14) continued			
Deoxycytidine	Deoxycytidine	Thymidine	Thymidine
Deoxyguanosine	Deoxyguanosine	Uric acid	Uric acid
Guanosine	Guanosine	Uridine	Uridine
Hypoxanthine	Hypoxanthine	Xanthine	Xanthine

Nucleotides (2)			
cAMP	Adenosine monophosphate, cyclic (cAMP)	cGMP	Guanosine monophosphate, cyclic (cGMP)

Organic acids (16)			
2,5-Furandi-carboxylic acid	Furan-2,5-dicarboxylic acid	4-Quinoline-carboxylic acid	4-Quinolinecarboxylic acid
2-Met-HipAcid	2-Methylhippuric acid	Abscisic acid	Abscisic acid
2-OH-2-Met-butyric acid	2-Hydroxy-2-methylbutyric acid	Argininic acid	Argininic acid
2-OH-Isobutyric acid	2-Hydroxyisobutyric acid	Bilirubin	Bilirubin
3-Guanidino-propionic acid	3-Guanidinopropionic acid	Biliverdin	Biliverdin
3-OH-HipAcid	3-Hydroxyhippuric acid	CMPE	3-Carboxy-4-methyl-5-propyl-2-furanpropionic acid
3-OH-Isobutyric acid	3-Hydroxyisobutyric acid	Glyceric acid	Glyceric acid
4-OH-HipAcid	4-Hydroxyhippuric acid	Nicotinuric acid	Nicotinuric acid

Phenolic acids (22)			
2-OH-Benzoic acid	2-Hydroxybenzoic acid	DOPAC	3,4-Dihydroxyphenylacetic acid
2-OH-Phenylacetic acid	2-Hydroxyphenylacetic acid	Homovanillic acid	Homovanillic acid
3-(3-OH-Phenyl)-propanoic acid	3-(3-Hydroxyphenyl)propanoic acid	HPHPA	3-(3-Hydroxyphenyl)-3-hydroxypropanoic acid

Phenolic acids (22) continued			
3,5-DiOH-Benzoic acid	3,5-Dihydroxybenzoic acid	OH-Phenyl-Lac	Hydroxyphenyllactic acid
3-OH-Phenylacetic acid	3-Hydroxyphenylacetic acid	Phenylacetic acid	Phenylacetic acid
3-OH-Phenylpyruvic acid	3-Hydroxyphenylpyruvic acid	Phenyl-Lac	Phenyllactic acid
4-OH-Benzoic acid	4-Hydroxybenzoic acid	Phenylpyruvic acid	Phenylpyruvic acid
4-OH-Phenylacetic acid	4-Hydroxyphenylacetic acid	t-p-Coumaric acid	trans-p-Coumaric acid
4-OH-Phenylpyruvic acid	4-Hydroxyphenylpyruvic acid	Vanillactic acid	Vanillactic acid
Benzoic acid	Benzoic acid	Vanillic acid	Vanillic acid
Desamino-Tyr	Desaminotyrosine	Vanillylmandelic acid	Vanillylmandelic acid

Phenoxy compounds (2)			
4-EPS	4-Ethylphenyl sulfate	Phenylglucuronide	Phenylglucuronide

Polyamines (7)			
Cadaverine	Cadaverine	N1-Ac-Spermine	N1-Acetylspermine
N1,N8-Di-Ac-Spermidine	N1,N8-Diacetylspermidine	N8-Ac-Spermidine	N8-Acetylspermidine
N1,N12-Di-Ac-Spermine	N1,N12-Diacetylspermine	N-Ac-Putrescine	N-Acetylputrescine
N1-Ac-Spermidine	N1-Acetylspermidine		

Pyridinecarboxylic acids (6)			
Isonicotinic acid	Isonicotinic acid	Quinaldic acid	Quinaldic acid
Kynurenic acid	Kynurenic acid	Quinolinic acid	Quinolinic acid
Picolinic acid	Picolinic acid	Xanthurenic acid	Xanthurenic acid

Sugars (7)			
3-Deoxy-glucosone	3-Deoxyglucosone	NeuAc	Acetylneuraminic acid
Fructose	Fructose	Ribose	Ribose
Glucose	Glucose	Threonic acid	Threonic acid
Mannose	Mannose		

Tricarboxylic acids (3)			
AconAcid	Aconitic acid	Isocitric acid	Isocitric acid
Citric acid	Citric acid		

Vitamins and cofactors (9)			
Biotin (B7)	Biotin (B7)	Pantothenic acid (B5)	Pantothenic acid (B5)
Choline	Choline	PMP	Pyridoxamine 5'-phosphate
Folic acid (B9)	Folic acid (B9)	Pyridoxine (B6)	Pyridoxine (B6)
Nicotinamide (B3)	Nicotinamide (B3)	Riboflavin (B2)	Riboflavin (B2)
Nicotinic acid (B3)	Nicotinic acid (B3)		

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