

Complete 296-Metabolite Panel

HMDB-anchored metabolite list organized by chemical class

The following tables present the complete 296-metabolite panel quantified by the Aristotle+ LC-MS/MS platform, organized by chemical class. Each metabolite is anchored to a Human Metabolome Database (HMDB) identifier for unambiguous chemical specification. The panel achieves 84% coverage of mapped human KEGG metabolic pathways.

Amino Acids & Derivatives (50 metabolites)

• 1-Methylhistidine	• 2-Aminoadipic acid	• 2-Aminobutyric acid
• 3-Aminobutyric acid	• 5-Aminolevulinic acid	• Acetylglycine
• Alanine	• Amino valerate	• Arginine
• Asparagine	• Aspartate	• Asymmetric dimethylarginine
• Caffeine	• Carnosine	• Citrulline
• Creatine	• Creatinine	• Cysteine
• Cystine	• DOPA	• Glutamic acid
• Glutamine	• Glycine	• Glycylproline
• Histidine	• Homocysteine	• Homoserine
• Hydroxyproline	• Isoleucine	• Isovalerylglycine
• Ketoleucine	• Leucine	• Lysine
• Methionine	• N-Acetylglutamine	• N-Acetylmethionine
• Norvaline	• Ornithine	• Phenylalanine
• Pterocollin	• Proline	• Pyroglutamic acid
• Sarcosine	• Serine	• Taurine
• Tetracaine	• Threonine	• Tryptophan
• Tyrosine	• Valine	

Organic Acids & TCA Intermediates (65 metabolites)

• 2,3-Dihydroxybenzoic acid	• 2-Furoic acid	• 2-Hydroxybenzoic acid
• 2-Hydroxyglutarate	• 2-Hydroxyphenylacetic acid	• 2-Ketobutyric acid
• 2-Methylglutaric acid	• 2-hydroxybutyric acid	• 3-Methyladipic acid
• 3-Phenyllactic acid	• 3-hydroxybutyric acid	• 4-Ethylbenzoic acid
• 4-Hydroxy-3-methylbenzoic acid	• 4-Hydroxybenzoic acid	• 4-Hydroxyphenylpyruvic acid
• 4-Methoxyphenylacetic acid	• Acetohydroxamic acid	• Aconitic acid
• Adipic acid	• Azelaic acid	• Benzoic acid
• Citraconic acid	• Citrate	• Ethylmalonic acid
• Ferulic acid	• Fumarate	• Gentisic acid
• Gibberellic acid	• Glucuronic acid	• Glutaconic acid
• Glutaric acid	• Glyceric acid	• Glycolic acid
• Glyoxylic acid	• Hippuric acid	• Homogentisic acid
• IsoCitrate	• Itaconic acid	• L-2-Hydroxyglutaric acid
• Lactate	• Leucic acid	• Levulinic acid
• Malate	• Maleic acid	• Malonic acid
• Mandelic acid	• Methylmalonic acid	• Muconic acid
• Oxaloacetic acid	• Oxoglutaric acid	• Phenylacetic acid
• Phenylglyoxylic acid	• Phenylpyruvic acid	• Phthalic acid
• Protocatechuic acid	• Pyruvate	• Sebacic acid
• Shikimic acid	• Suberic acid	• Succinate
• Tartaric acid	• Vanillic acid	• m-Coumaric acid

- meso-Tartaric acid
- p-Coumaric acid

Nucleotides, Purines & Pyrimidines (38 metabolites)

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|---------------------|--------------------|--------------------|
| • 1-Methyladenosine | • 2-Deoxyadenosine | • 2-Deoxyuridine |
| • 2-deoxyguanosine | • 5-Methylcytidine | • ADP |
| • ADP ribose | • AMP | • ATP |
| • Adenine | • Adenosine | • Adenylosuccinate |
| • Cytidine | • Cytosine | • DCDP |
| • DCTP | • DUMP | • Deoxycytidine |
| • GDP | • Guanine | • Guanosine |
| • Hypoxanthine | • Inosine | • NADP |
| • NADPH | • Neopterin | • SAICAR |
| • UDP | • UDP-GlcNAc | • Uracil |
| • Urate | • Uridine | • Xanthine |
| • Xanthosine | • cADPR | • cGMP |
| • dTMP | • dUTP | |

Lipids, Fatty Acids & Acylcarnitines (24 metabolites)

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|------------------------|----------------------------|------------------------------|
| • 3-Hydroxybutyryl-CoA | • 3-Hydroxyisovaleric acid | • 3-Methyl-2-oxovaleric acid |
| • Acetyl-CoA | • Acetylcarnitine | • Capric acid |
| • Caprylic acid | • Carnitine | • Decanoylcarnitine |
| • Heptadecanoic acid | • Hexanoic acid | • Isobutyric acid |
| • Isobutyryl-CoA | • Isovaleric acid | • Lauric acid |
| • Malonyl-CoA | • Myoinositol | • Myristic acid |
| • PGE2 | • Palmitic acid | • Pentadecanoic acid |
| • Stearic acid | • Valeric acid | • pregnenolone sulfate |

Carbohydrates & Sugar Phosphates (40 metabolites)

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|---------------------------|--------------------------|------------------------------------|
| • 3-Phosphoglyceric acid | • 6-Phosphogluconic acid | • Adonitol |
| • Cellobiose | • D-Galacturonic acid | • D-Mannitol |
| • D-Ribose 5-phosphate | • Dihydroxyacetone | • Dulcitol |
| • Erythrose | • Fructose | • Fructose 1,6-bisphosphate |
| • Galactonic acid | • Gluconic acid | • Glucosamine |
| • Glucosamine 6-phosphate | • Glucose | • Glucose 1,6-bisphosphate |
| • Glucose 1-phosphate | • Glucose 6-phosphate | • Glyceraldehyde 3-phosphate |
| • L-(+)-Arabinose | • L-Arabitol | • Lactose |
| • Mannose | • Mannose 6-phosphate | • Methyl alpha-D-galactopyranoside |
| • Mucic acid | • N-Acetyl-D-Glucosamine | • N-Acetyl-D-galactosamine |
| • N-Acetylneuraminic acid | • PEP | • Raffinose |
| • Ribose | • Sorbitol | • Sucrose |
| • Trehalose | • Xylitol | • Xylose |
| • Xylulose-5-phosphate | | |

Vitamins & Cofactors (17 metabolites)

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|---------------------|-------------------------------|--------------------|
| • 4-Pyridoxic acid | • 6-Hydroxynicotinic acid | • Biotin |
| • Dihydrofolic acid | • Folic acid | • Folinic acid |
| • L-Ascorbic acid | • NAD | • NADH |
| • Nicotinamide | • Nicotinamide mononucleotide | • Nicotinic acid |
| • Nicotinuric acid | • Nonadecanoic acid | • Pantothenic acid |
| • Pyridoxine | • Vitamin D3 | |

Neurotransmitters & Neuroactive (30 metabolites)

• 3-Indolepropionic acid	• 3-hydroxyanthranilic acid	• 3-hydroxykynurenine
• 4-Aminobutyric acid	• 4-Imidazoleacetic acid	• 5-Hydroxyindoleacetic acid
• 5-Hydroxytryptophan	• Acetylcholine	• Anthranilic acid
• Dopamine	• Epinephrine	• Histamine
• Homovanillic acid	• Imidazole	• Indole
• Indole-3-acetic acid	• Indole-3-lactic acid	• Indole-3-pyruvic acid
• Kynurenic acid	• Kynurenine	• Melatonin
• Metanephrine	• Methylhistamine	• Normetanephrine
• Picolinic acid	• Quinolinic acid	• Serotonin
• Tryptamine	• Urocanic acid	• Xanthurenic acid

Redox & Antioxidant Markers (6 metabolites)

• 3-Nitrotyrosine	• Acetylcysteine	• Cystamine
• Glutathione	• Methylguanidine	• Oxidized Glutathione

Polyamines & Biogenic Amines (4 metabolites)

• Agmatine	• Cadaverine	• Putrescine
• Spermidine		

One-Carbon & Methylation (7 metabolites)

• Adenosyl-L-homocysteine	• Betaine	• Choline
• Dimethylglycine	• Glycocyamine	• Phosphocreatine
• TMAO		

Other Metabolites (15 metabolites)

• 2-Phenylglycinol	• 2-Pyrrolidinone	• 4-Aminophenol
• 4-Hydroxybenzaldehyde	• Acetamide	• Acetoacetate
• Allopurinol	• Amiloride	• Methyl succinate
• N,N-Dicyclohexylurea	• N-Acetylmuramic Acid	• Naproxen
• Phenylbutazone	• Propranolol	• Thymol

Total metabolites: 296