Target Analysis for Human/Animal Serum/Plasma Samples by Chemical Isotope Labeling LC-MS

TMIC
The Metabolomics Innovation Center

Provided by TMIC-Li Node

Features

Quantitative Analysis: Accurate and Precise Relative Quantification

- Unique isotope labeled internal standard for each metabolite
- Amount/concentration comparisons between groups

High Metabolite Coverage: Multiple Pathway Analysis

- One single assay for analyzing many metabolites from various pathways
- Combining up to three assays to achieve very high coverage

Flexibility and Affordability: Customizable Assays

- Easy to add more metabolites of interest without adding extra cost
- As low as $120 CAD per sample

Assay List

Amino Acids & Derivatives – Core Panel	114 Metabolites
Amino Acids & Derivatives – Full Panel	175 Metabolites
Dipeptides & Tripeptides	145 Metabolites
Polyamines	5 Metabolites
Neurotransmitters	6 Metabolites
Short & Medium Chain Fatty Acids	18 Metabolites
Bile Acids	19 Metabolites
Steroid Hormones	24 Metabolites
Nucleoside Metabolism – Core Panel	25 Metabolites
Nucleoside Metabolism – Full Panel	37 Metabolites
Energy Metabolism – Core Panel	23 Metabolites
Energy Metabolism – Full Panel	56 Metabolites
Tryptophan Metabolism	32 Metabolites
Phenylalanine Metabolism	31 Metabolites
Alanine, Aspartate and Glutamate Metabolism	11 Metabolites
Tyrosine Metabolism	43 Metabolites
Glycine, Serine and Threonine Metabolism	24 Metabolites
Valine, Leucine and Isoleucine Metabolism	10 Metabolites
Arginine and Proline Metabolism	45 Metabolites
Lysine Metabolism	28 Metabolites
Cysteine and Methionine Metabolism	24 Metabolites
Histidine Metabolism	19 Metabolites
Benzoate Metabolism	16 Metabolites

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Amino Acids & Derivatives – Core Panel (114 Metabolites)

Alanine
Arginine
Asparagine
Aspartic acid
Cysteine
Glutamic acid
Glutamine
Glycine
Histidine
Isoleucine
Leucine
Lysine
Methionine
Phenylalanine
Proline
Serine
Threonine
Tryptophan
Tyrosine
Valine
Homoserine
Ornithine
Citrulline
3,4-Dihydroxy-L-phenylalanine
N-Acetylornithine
N6-(L-1,3-Dicarboxypropyl)-L-lysine
Cystine
L-Cysteic acid
Allocystathionine
3-Sulfino-L-alanine
Meso-2,6-Diaminoheptanedioic Acid
Aminoadipic acid
O-Acetyl-L-serine hydrochloride
O-Acetyl-Homoserine
1-Methylhistidine
4-Hydroxyproline
L-Glutamate 5-semialdehyde
Allysine
Nopaline
Kynurenine
Homocystine
4-Oxoproline
Homoarginine
Norleucine
Cystathionine
2-Aminobutyric acid
Homocitrulline
Formylkynurenine
N6-Acetyl-Lysine
N(6)-Methyllysine
Methionine Sulfoxide
3-Hydroxykynurenine
2,4-Diaminobutyric acid
cis-4-Hydroxy-D-proline
Threo-3-Methylaspartic Acid
Gamma-Glutamylalanine
2-Amino-6-Oxoheptanedioic Acid
Serine-Phosphoethanolamine
(2R,4S)-2,4-Diaminopentanoic Acid
D-Lysopine
2-Aminoadipate 6-Semialdehyde
D-Octopine
3-Hydroxy-L-proline
2-(3-Carboxy-3-Aminopropyl)-L-Histidine
4-(L-Alanin-3-yl)-2-hydroxy-cis,cis-muconate 6-semialdehyde
3-Hydroxy-L-proline
Gamma-Glutamylglutamate
Beta-Alanyl-L-Lysine
L-Allothreonine
S-Glutathionyl-L-cysteine
P-Hydroxyphenylacetylglycine
5-Hydroxy-N-Formylkynurenine
5-Hydroxykynurenine
2-Amino-5-Oxohexanoic Acid
5-Hydroxyindoleacetylglycine
4-Hydroxyglutamate Semialdehyde
L-erythro-4-Hydroxyglutamic acid
Ectoine
N-Ethylglycine
N-Methyl Aspartic Acid
gamma-L-Glutamylputrescine
5-Hydroxyectoine
Isoglutamine
5-Hydroxylysine
L-Homophenylalanine
(2S,5S)-trans-Carboxymethylproline
3-Hydroxy-Proline
(2R,3R)-3-Methylornithine
(2R,3R)-3-Methylglutamyl-5-Semialdehyde-N6-Lysine
Gamma-Glutamyltyramine
Gamma-L-Glutamyl-L-2-Aminobutyric Acid
Ophthalmic acid
3-Amino-2-Piperidone
N-Alpha-Acetyllysine
3-Methylhistidine
Cysteineglutathione disulfide
N-Acetyl-Tyrosine
2-Aminooctanoic Acid
3-Nitrotyrosine
3-Phenylpropionylglycine
N-Acetyl-L-Arginine
Homocysteinesulfinic acid
3-Mercaptolactate-Cysteine Disulfide
L-beta-aspartyl-L-serine
L-glycyl-L-hydroxyproline
gamma-Glutamyllysine
L-Tyrosine O-sulfate
N2-Acetyl-L-Kynurenine
N-Acetyl-5-Hydroxy-L-tryptophan
N-Acetyl-L-Cystine
N-Acetyl-N(Omega)-Hydroxyarginine
N2-Acetyl-5'-Hydroxykynurenine
N5-Acetyl-Ornithine
O-Methyl-L-threonine

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Amino Acids & Derivatives – Full Panel (175 Metabolites)

Alanine
Arginine
Asparagine
Aspartic acid
Cysteine
Glutamic acid
Glutamine
Glycine
Histidine
Isoleucine
Leucine
Lysine
Methionine
Phenylalanine
Proline
Serine
Threonine
Tryptophan
Tyrosine
Valine
Homoserine
Ornithine
Homocysteine
Citrulline
3,4-Dihydroxy-L-phenylalanine
N-Acetylornithine
N6-(L-1,3-Dicarboxypropyl)-L-lysine
Cystine
L-Cysteic acid
Allocystathionine
3-Sulfino-L-alanine
5-Hydroxy-L-tryptophan
Meso-2,6-Diaminoheptanedioic Acid
L-Arogenic Acid
Aminomalonic acid
Aminoadipic acid
O-Acetyl-L-serine hydrochloride
N6-Hydroxy-L-lysine
N-AcetyAspartic Acid
N-Formyl-L-aspartic acid
O-Acetyl-Homoserine
1-Methylhistidine
4-Hydroxyproline
L-Glutamate 5-semialdehyde
N-Acetyl-Glutamate 5-Semialdehyde
Allysine
Nopaline
Kynurenine
L-Norvaline
Homocystine
Thyroxine
4-Oxoproline
Homoarginine
Norleucine
Thiocysteine
(S)-Ureidoglycine
Cystathionine
2-Aminobutyric acid
Homocitrulline
Formylkynurenine
N6-Acetyl-Lysine
N(6)-Methyllysine
Methionine Sulfoxide
Acetyl-Histidine
N-Formylmethionine
3-Hydroxykynurenine
2,4-Diaminobutyric acid
N2-Succinyl-L-arginine
cis-4-Hydroxy-D-proline
N-Acetyl-Phenylalanine
Threo-3-Methylaspartic Acid
Gamma-Glutamylalanine
2-Amino-6-Oxoheptanedioic Acid
Serine-Phosphoethanolamine
(2R,4S)-2,4-Diaminopentanoic Acid
D-Lysopine
2-Aminoadipate 6-Semialdehyde
D-Octopine
Phenylacetylglutamine
3-Hydroxy-L-proline
2-(3-Carboxy-3-Aminopropyl)-L-Histidine
4-(L-Alanin-3-yl)-2-hydroxy-cis,cis-muconate 6-semialdehyde
1-(5'-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole
3-Hydroxy-L-proline
Gamma-Glutamylglutamate
Beta-Alanyl-L-Lysine
L-Allothreonine
S-Glutathionyl-L-cysteine
Hydantoin-5-propionic acid
P-Hydroxyphenylacetylglycine
Phenylacetylglycine
5-Hydroxy-N-Formylkynurenine
5-Hydroxykynurenine
2-Amino-5-Oxohexanoic Acid
5-Hydroxyindoleacetylglycine
N-Succinyl-L-glutamate 5-semialdehyde
4-Hydroxyglutamate Semialdehyde
L-erythro-4-Hydroxyglutamic acid
Stizolobic acid
Ectoine
Acetylcysteine
N-Ethylglycine
N-Methyl Aspartic Acid
N-Acetylaspartylglutamic Acid
gamma-L-Glutamylputrescine
Iminoglycine
5-Hydroxyectoine
Isoglutamine
5-Hydroxylysine
L-Homophenylalanine
(2S,5S)-trans-Carboxymethylproline
N-Nitrosoproline
3-Hydroxy-Proline
N(Alpha)-Acetyl-L-2,4-Diaminobutyric Acid
(2R,3R)-3-Methylornithine
(2R,3R)-3-Methylglutamyl-5-Semialdehyde-N6-Lysine
beta-Citryl-L-glutamic acid
Gamma-Glutamyltyramine
Gamma-L-Glutamyl-L-2-Aminobutyric Acid
Ophthalmic acid
3-Amino-2-Piperidone
2-Methylbutyrylglycine
2-Furoylglycine
N-Alpha-Acetyllysine
3-Methylcrotonylglycine
3-Methylhistidine
Acetylglycine
Cysteineglutathione disulfide
Hexanoylglycine
Isobutyrylglycine
Propionylglycine
N-Acetyl-Tyrosine
2-Aminooctanoic Acid
3-Nitrotyrosine
3-Phenylpropionylglycine
N-Acetyl-DL-serine
N-Acetyl-L-Arginine
Dityrosine
Homocysteinesulfinic acid
3-Mercaptolactate-Cysteine Disulfide
Vinylacetylglycine
L-beta-aspartyl-L-serine
L-glycyl-L-hydroxyproline
N-Acetyl-Valine
1-(1,2,3,4,5-Pentahydroxypent-1-yl)-1,2,3,4-tetrahydro-beta-carboline-3-carboxylic acid
N-Decanoylglycine
N-Nonanoylglycine
Tridecanoylglycine
N-Acetyltryptophan
Gamma-Glutamylaspartic Acid
gamma-Glutamyllysine
S-Cysteinosuccinic Acid
L-Tyrosine O-sulfate
N2-Acetyl-L-Kynurenine
N-Acetyl-Alanine
N-Formyl-DL-phenylalanine
N-Formyltryptophan
N-Acetyl-(S)-2-Aminobutanoic acid
N-Acetyl-5-Hydroxy-L-tryptophan
N-Acetyl-Gamma-Glutamyl-2-Aminobutyric Acid
N-Acetyl-Hydroxyproline
N-Acetyl-L-2-Amino-3-oxobutanoic acid
N-Acetyl-L-2-Aminoadipic acid
N-Acetyl-L-Cystine
N-Acetyl-N(Omega)-Hydroxyarginine
N-Acetyl-N(pi)-Methyl-L-histidine
N-Acetyl-O-Phospho-4-hydroxy-L-threonine
N-Acetyl-Ophthalmic Acid
N2-Acetyl-(2R,4S)-2,4-Diaminopentanoic acid
N2-Acetyl-5'-Hydroxykynurenine
N2-Acetyl-Cysteinyldopa
N4-Acetyl-(2R,4S)-2,4-Diaminopentanoic Acid
N5-Acetyl-Ornithine
O-Methyl-L-threonine
Tyrosine O-glucuronide

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Dipeptides & Tripeptides (145 Metabolites)

Alanyl-Alanine
Alanyl-Aspartic Acid
Alanyl-Glutamine
Alanyl-Glycine
Alanyl-Leucine
Alanyl-Proline
Arginyl-Glycine
Arginyl-Proline
Asparaginyl-Proline
Aspartyl-Glutamine
Aspartyl-Glycine
Aspartyl-Histidine
Aspartyl-Leucine
Aspartyl-Lysine
Aspartyl-Proline
Aspartyl-Threonine
Aspartyl-Valine
Glutaminyl-Aspartate
Glutaminyl-Glutamate
Glutaminyl-Proline/Prolyl-Glutamine
Glutaminyl-Threonine
Glutamyl-Asparagine
Glutamyl-Glycine
Glutamyl-Isoleucine
Glutamyl-Methionine
Glutamyl-Serine
Glutamyl-Valine
Gly-Norvaline
Glycyl-Alanine
Glycyl-Glutamine
Glycyl-Glycine
Glycyl-Phenylalanine
Glycyl-Serine
Glycyl-Valine
Histidinyl-Alanine
Histidinyl-Aspartate
Histidinyl-Glutamate
Histidinyl-Tryptophan
Isoleucyl-Alanine
Isoleucyl-Glycine
Isoleucyl-Lysine
Isoleucyl-Phenylalanine
Isoleucyl-Valine
Leucyl-Alanine
Leucyl-Aspartate
Leucyl-Glutamate
Leucyl-Glutamine
Leucyl-Glycine
Leucyl-Leucine
Leucyl-Threonine
Lysyl-Alanine
Lysyl-Glutamate
Lysyl-Glutamine
Lysyl-Glycine
Lysyl-Leucine/Leucyl-Lysine
Lysyl-Proline
Lysyl-Serine
Lysyl-Tyrosine
Lysyl-Valine
Methionyl-Alanine
Methionyl-Isoleucine
Phenylalanyl-Alanine
Phenylalanyl-Aspartate
Phenylalanyl-Glutamate
Phenylalanyl-Glycine
Phenylalanyl-Phenylalanine
Phenylalanyl-Serine
Phenylalanyl-Threonine
Phenylalanyl-Tryptophan
Phenylalanyl-Valine
Prolyl-Alanine
Prolyl-Arginine
Prolyl-Asparagine/Asparaginyl-Proline
Prolyl-Aspartate
Prolyl-Glutamate
Prolyl-Glycine
Prolyl-Histidine
Prolyl-Isoleucine
Prolyl-Leucine
Prolyl-Lysine
Prolyl-Methionine
Prolyl-Proline
Prolyl-Serine
Prolyl-Threonine
Prolyl-Tryptophan
Prolyl-Tyrosine
Seryl-Alanine
Seryl-Aspartic Acid
Seryl-Cysteine
Seryl-Glutamate
Seryl-Isoleucine
Seryl-Threonine
Seryl-Tyrosine
Threoninyl-Cysteine
Threoninyl-Glutamate
Threoninyl-Glutamine
Threoninyl-Phenylalanine
Tryptophyl-Glycine
Tyrosyl-Asparagine
Tyrosyl-Aspartate
Tyrosyl-Glutamate
Tyrosyl-Glutamine
Tyrosyl-Glycine
Tyrosyl-Histidine
Tyrosyl-Lysine
Tyrosyl-Methionine
Valyl-Alanine
Valyl-Arginine
Valyl-Glutamine
Valyl-Glycine
Valyl-Isoleucine
Valyl-Leucine
Valyl-Lysine
Valyl-Threonine
Alanyl-Glutamic Acid
Asparaginyl-Alanine
Asparaginyl-Hydroxyproline
Asparaginyl-Methionine
Asparaginyl-Valine
Cysteinyl-Proline
Gamma-glutamyl-ornithine
Glutaminylmethionine
Glycyl-Lysine
Histidinyl-Hydroxyproline
Hydroxyprolyl-Gamma-glutamic acid
Hydroxyprolyl-Methionine
Hydroxyprolyl-Proline
Hydroxyprolyl-Serine
Hydroxyprolyl-Valine
Isoleucyl-Hydroxyproline
L-Beta-Aspartyl-L-Glycine
L-Cysteinylglycine disulfide
L-alpha-Aspartyl-L-hydroxyproline
L-alpha-glutamyl-L-hydroxyproline
Leucyl-Hydroxyproline
Methionyl-Glutamic Acid
Prolyl-Gamma-glutamic acid
Prolyl-Glutamine
Prolyl-Hydroxyproline
Prolyl-Valine
Serinyl-Hydroxyproline
Seryl-Proline
Serylglycine
gamma-Glutamyl-Glycine
gamma-Glutamyl-Proline

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Polyamines (5 Metabolites)

1,3-Diaminopropane	Cadaverine	N8-Acetylspermidine
1,4-diaminobutane	Spermidine	

Neurotransmitters (6 Metabolites)

Dopamine	Histamine	Tyramine
Gamma-Aminobutyric Acid	Serotonin	Octopamine

Short & Medium Chain Fatty Acids (18 Metabolites)

Acetic Acid	Isovaleric Acid	8-Methyl-6-nonenoic acid
Acrylic Acid	Valeric Acid	Citronellic Acid
Propionic Acid	Hexanoic Acid	Capric Acid
Butyric Acid	Isocaproic Acid	Hendecanoic Acid
Tiglic Acid	Octanoic Acid	5-Dodecenoic acid
2-Methylbutanoic acid	Geranic acid	Lauric Acid

Bile Acids (19 Metabolites)

Cholic Acid	Gamma-Muricholic Acid	9(11), (5beta)-Cholenic Acid-3alpha-Ol-12-One
Glycocholic Acid	Isolithocholic Acid	3beta-Hydroxy-delta5-cholenic acid
Chenodeoxycholic Acid	Allochenodeoxycholic acid/Isochenodeoxycholic acid/Isoursodeoxycholic acid	5Alpha-Cholanic Acid-3Alpha-Ol-6-One
Lithocholic Acid	Allocholic acid	5beta-Cholanic acid-7alpha-ol-3-one
Deoxycholic Acid	5-Beta-Cholanic Acid-3Beta, 12Alpha-Diol	Glycoursodeoxycholic acid-3-sulfate
Glycodeoxycholic Acid	Avideoxycholic acid	Nordeoxycholic acid
Glycochenodeoxycholic Acid	3Beta-Hydroxy-5-Cholenoic Acid	
Ursodeoxycholic Acid	Glycoursodeoxycholic Acid	
7Alpha-Hydroxy-3-Oxo-4-Cholestenoic Acid		
Alpha-Muricholic Acid		

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Steroid Hormones (24 Metabolites)

Testosterone	Estrone glucuronide	18-Hydroxycorticosterone 21-O-sulfate
Cortisol	11-Dehydrocorticosterone 21-O-glucuronide	Androstenediol 3-O-sulfate
Cortisone	11-Deoxycortisol 21-O-glucuronide	Cortisol 21-O-sulfate
18-Hydroxycorticosterone	11-Deoxycortisol 21-O-sulfate	Cortol 3-O-sulfate
Dehydroepiandrosterone	16-Hydroxyestrone 3-O-sulfate	Dihydrotestosterone 17-O-sulfate
Dihydrotestosterone	16alpha-Hydroxyestrone 3-O-glucuronide	Estriol 17-O-sulfate
5b-Androsterone	17alpha,21-Dihydroxypregnenolone 3-O-sulfate	Urocortisol 3-O-sulfate
Dehydroepiandrosterone sulfate		
2-Hydroxyestrone		
Cortolone		
Estradiol-17beta 3-glucuronide		

Nucleoside Metabolism – Core Panel (25 Metabolites)

Glyoxylic Acid	Guanosine	1-(5'-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole
Beta-Alanine	Cytidine	3-Aminoisobutanoic acid
Uracil	Oxalureic acid	3-Oxo-3-ureidopropanoic acid
Thymine	Deoxycytidine	Aminoacrylic acid
Guanine	Hydracrylic Acid	Ureidoacrylic Acid
Hypoxanthine	Oxamic acid	N-Acetyl-5-Amino-4-imidazole carboxylic acid
Uridine	Carbamic acid	
Uric acid	(S)-Ureidoglycine	
Malonic acid	Methylmalonic acid	
Xanthine	3-Ureidopropionic Acid	

Nucleoside Metabolism – Full Panel (37 Metabolites)

Glyoxylic Acid	Cytidine	3-Aminoisobutanoic acid
Beta-Alanine	Deoxyuridine	Deoxyinosine
Uracil	Deoxyadenosine	3-Oxo-3-ureidopropanoic acid
Thymine	Oxalureic acid	Aminoacrylic acid
Adenosine	Deoxycytidine	Ureidoacrylic Acid
3-Oxopropanoic acid	Hydracrylic Acid	N-Acetyl-5-Amino-4-imidazole carboxylic acid
Guanine	Oxamic acid	
Hypoxanthine	Carbamic acid	N-Acetyl-Adenosine
Inosine	Pseudouridine	N-Acetyl-Deoxyadenosine
Uridine	(S)-Ureidoglycine	N-Acetyl-Deoxyguanosine
Uric acid	Methylmalonic acid	N-Acetyl-Guanosine
Malonic acid	3-Ureidopropionic Acid	N-Acetyl-Deoxycytidine
Xanthine	1-(5'-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole	
Guanosine		

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Energy Metabolism – Core Panel (23 Metabolites)

Succinic Acid	2-Dehydro-3-deoxy-galactonic acid/2-Dehydro-3-deoxy-D-gluconic acid	Oxalosuccinic Acid
Fumaric Acid/Maleic acid	Mesaconic Acid	Xylonic Acid
Citric Acid / Isocitric Acid	3-Ethylmalic acid	4-Methyl-L-Glutamic Acid
Glycolic Acid	3-Oxalomalic Acid	Cis-(Homo)2-Aconitic Acid
Propionic Acid	(R)-2-Ethylmalic Acid	Gamma-Glutamyltyramine
Methylamine	Threo-3-Methylaspartic Acid	2-Methyl-Trans-Aconitic Acid/(Z)-But-2-Ene-1,2,3-Tricarboxylic Acid
4-Methylene-Glutamic Acid	2-Hydroxyethylenedicarboxylic Acid	N-Acetyl-Dihydrofolic Acid
D-Fructuronic acid/D-Tagaturonic acid		
4-Methylene-Glutamine		

Energy Metabolism – Full Panel (56 Metabolites)

Oxoglutaric acid	(R)-3,3-Dimethylmalic acid	acid
Succinic Acid	Trimethylamine N-oxide	N-((R)-Pantothenoyl)-L-cysteine
Glycerol	4-Methylene-Glutamine	(4S)-4,6-Dihydroxy-2,5-dioxohexanoic acid
Fumaric Acid/Maleic acid	2-Dehydro-3-deoxy-galactonic acid/2-Dehydro-3-deoxy-D-gluconic acid	Hydroxyacetone
Citric Acid / Isocitric Acid	Ethylene glycol	Oxalosuccinic Acid
Glycolic Acid	Mesaconic Acid	Xylonic Acid
Propionic Acid	Propan-2-ol	4-Hydroxy-4-methylglutamic acid
D-(+)-Xylose	Arabitol	4-Methyl-L-Glutamic Acid
Methylamine	3-Ethylmalic acid	(R)-(Homo)2-citric acid
Glycolaldehyde	3-Oxalomalic Acid	7-Oxoheptanoic acid
D-Ribulose	2-Methylcitric acid	(-)-threo-Iso(homo)2-citric acid
D-Xylulose	Digalacturonic acid	(R)-(Homo)3-citric acid
Lyxose	(R)-2-Ethylmalic Acid	(-)-threo-Iso(homo)3-citric acid
Propanal	Threo-3-Methylaspartic Acid	7,8-Didemethyl-8-hydroxy-5-deazariboflavin
(R)-Pantoic acid	2-Dehydro-3-deoxy-D-xylonic acid	Cis-(Homo)2-Aconitic Acid
Propane-1,2-diol	2-Hydroxyethylenedicarboxylic Acid	Gamma-Glutamyltyramine
3-Dehydro-L-gulonic acid	2,3-Dihydroxy-3-methylbutanoic acid	2-Methyl-Trans-Aconitic Acid/(Z)-But-2-Ene-1,2,3-Tricarboxylic Acid
4-Methylene-Glutamic Acid	5-Dehydro-4-deoxy-D-glucuronic	N-Acetyl-Dihydrofolic Acid
Pantetheine		
D-Fructuronic acid/D-Tagaturonic acid		
(R)-4-Dehydropantoic acid		

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Tryptophan Metabolism (32 Metabolites)

2-Aminobenzoic Acid	4,8-Dihydroxyquinoline	semialdehyde
3-Hydroxyanthranilic Acid	5-Hydroxy-L-tryptophan	N-Acetyl-3-Hydroxyanthranilic acid
5-Hydroxyindole- 3-Acetic Acid	5-Hydroxy-N-Formylkynurenine	N-Acetyl-5-Hydroxy-L-tryptophan
Indoleacetic Acid	5-Hydroxyindoleacetaldehyde	N-Acetyl-Formyl-5-hydroxykynurenamine
Indolelactic Acid	5-Hydroxyindoleacetylglycine	N-Acetylindoxyl
Kynurenine	5-Hydroxykynurenamine	N2'-Acetyl-3'-Hydroxykynurenamine
Serotonin	5-Hydroxykynurenine	N2-Acetyl-5'-Hydroxykynurenine
2-Amino-3-Carboxymuconate Semialdehyde	Formyl-5-hydroxykynurenamine	N2-Acetyl-L-Kynurenine
2-Aminomuconate semialdehyde	Formylanthranilic Acid	N3-Acetyl-3'-Hydroxykynurenamine
2-Aminomuconic Acid	Formylkynurenine/L-Formylkynurenine	
3-Hydroxykynurenine	Indoxyl	
3-Methoxyanthranilic Acid	N-Acetyl-2-Aminomuconate	

Phenylalanine Metabolism (31 Metabolites)

3-(2-Hydroxyphenyl)Propionic Acid	Salicylic acid	N-Acetyl-Vanillylamine
3-(3-Hydroxyphenyl)Propionic Acid	Vanillin	cis-3-(3-Carboxyethenyl)-3,5-cyclohexadiene-1,2-diol
3-Phenyllactic Acid	2-Hydroxy-2,4-pentadienoic acid	3-Hydroxybenzoic Acid
Benzoic Acid	2-Hydroxy-3-phenylpropenoic acid	Protocatechuic Acid
Hippuric Acid	2-Hydroxy-6-ketononatrienedioic acid	Shikimic Acid
Hydrocinnamic Acid / 3-Methylphenylacetic Acid	2-Hydroxy-6-oxonona-2,4-diene-1,9-dioic acid	(4R,5R)-4,5-Dihydroxycyclohexa-1(6),2-Diene-1-Carboxylic Acid
Hydroxyphenylacetic Acid	3-(2,3-Dihydroxyphenyl)propanoic acid	2-Benzylmalic Acid
N-Acetyl-Phenylalanine	8-Methyl-6-nonenoic acid	2-Oxo-4-Phenylbutyric Acid
Phenylacetic Acid	Cis-3-(Carboxy-Ethyl)-3,5-Cyclo-Hexadiene-1,2-Diol	3-Dehydroquinic Acid
Phenylacetylglutamine		L-Arogenic Acid
Phenylacetylglycine		L-Homophenylalanine
Phenylalanine		

Alanine, Aspartate and Glutamate Metabolism (11 Metabolites)

Alanine	Succinic acid semialdehyde	N-AcetyAspartic Acid
Asparagine	1-Pyrroline-5-Carboxylic Acid	N-Acetylaspartylglutamic Acid
Gamma-Aminobutyric Acid	2-Oxosuccinamic Acid	beta-Citryl-L-glutamic acid
N-Acetyl-Alanine	Ketoglutarate	

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Tyrosine Metabolism (43 Metabolites)

2,5-Dihydroxybenzoic Acid	semialdehyde	5,6-Indolequinone-2-carboxylic acid
3,4-Dihydroxybenzeneacetic Acid	2-Hydroxyhepta-2,4-dienedioic acid	5-Carboxymethyl-2-hydroxymuconic acid
3,4-Dihydroxymandelic Acid	3,4-Dihydroxy-L-phenylalanine	Fumarylacetoacetic Acid/4-Maleylacetoacetate
3-Hydroxyphenylacetic Acid	3,4-Dihydroxymandelaldehyde	Gentisate Aldehyde
4-Hydroxyphenylacetic Acid	3,4-Dihydroxyphenylacetaldehyde	Hydroquinone
Dopamine	3-(3,4-Dihydroxyphenyl)lactic acid	Maleylpyruvic acid/3-Fumarylpyruvic acid
Phenol	3-(3,4-Dihydroxyphenyl)pyruvic acid	N-Acetyl-2-Carboxy-2,3-dihydro-5,6-dihydroxyindole
Thyroxine	3-Amino-3-(4-hydroxyphenyl)propanoic acid	N-Acetyl-3-Methoxytyramine
Tyramine	3-Methoxy-4-Hydroxyphenylethyleneglycol	N-Acetyl-Dopamine
Vanillylmandelic acid	3-Methoxy-4-hydroxyphenylacetaldehyde	N-Acetyl-L-Metanephrine
2,4-Dihydroxyhept-2-enedioic acid	4-(L-Alanin-3-yl)-2-hydroxy-cis,cis-muconate 6-semialdehyde	N-Acetyl-L-Noradrenaline
2-Carboxy-2,3-Dihydro-5,6-Dihydroxyindole	4-Chlorophenylacetic acid	N-Acetyl-Tyramine
2-Hydroxy-3-(4-Hydroxyphenyl)Propenoic Acid	4-Hydroxyphenylacetaldehyde	N2-Acetyl-Cysteinyldopa
2-Hydroxy-3-(4-hydroxyphenyl)propenoate O-sulfate	5,6-Dihydroxyindole	P-Hydroxyphenylacetylglycine
2-Hydroxy-5-carboxymethylmuconate		Stizolobic acid

Glycine, Serine and Threonine Metabolism (24 Metabolites)

1,3-Diaminopropane	N-Acetyl-DL-serine	Cysteine
2,4-Diaminobutyric acid	Sarcosine	Ectoine
Acetylcysteine	Serine	Hydroxypyruvic Acid
Aminolevulinic Acid	Threonine	L-Allothreonine
Choline	Tryptophan	N(Alpha)-Acetyl-L-2,4-Diaminobutyric Acid
Creatine	(R)-1-Aminopropan-2-Ol	N-Acetyl-L-2-Amino-3-oxobutanoic acid
Cystathionine	5,10-Methylenetetrahydrofolic Acid	
Guanidoacetic acid	5-Hydroxyectoine	
Homoserine	Aminoacetone	

Valine, Leucine and Isoleucine Metabolism (10 Metabolites)

3-Hydroxyisobutyric acid	Methyloxovaleric acid	3-Hydroxy-3-Methyl-2-Oxobutanoic Acid
3-Hydroxyisovaleric Acid	Valine	D-erythro-3-Methylmalic acid
L-Isoleucine	N-Acetyl-Valine	
Leucine	(R/S)-2-Methylmalic Acid	

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Arginine and Proline Metabolism (45 Metabolites)

Arginine	acid	L-erythro-4-Hydroxyglutamic acid
Aspartic acid	3-Hydroxy-L-proline	N-Acetyl-2-Oxo-4-hydroxy-5-aminovaleric acid
Citrulline	3-Hydroxy-Proline	N-Acetyl-5-Amino-2-Oxopentanoic Acid
Glutamine	4-Acetamidobutanoic acid	N-Acetyl-Hydroxyproline
L-Glutamic Acid	4-Aminobutyraldehyde	N-Acetyl-N(Omega)-Hydroxyarginine
Ornithine	4-Guanidinobutanal	N-Carbamoylsarcosine
N-Acetyl-Glutamate 5-Semialdehyde	4-Guanidinobutanoic acid	N-Succinyl-L-glutamate 5-semialdehyde
N-Acetyl-L-Arginine	4-Hydroxyglutamate Semialdehyde	N2-Succinyl-L-arginine
N-Acetylornithine	4-Oxoproline	Nopaline
N5-Acetyl-Ornithine	5-Amino-2-Oxopentanoic Acid	Phosphocreatine
1,4-diaminobutane	5-Guanidino-2-Oxopentanoic Acid	gamma-L-Glutamylputrescine
4-Hydroxyproline	D-Octopine	p-Coumaroylagmatine
Proline	Feruloylputrescine	p-Coumaroylputrescine
Spermidine	Gamma-Glutamyl-Gamma-Aminobutyraldehyde	
cis-4-Hydroxy-D-proline	L-1-Pyrroline-3-hydroxy-5-carboxylic acid	
1-Pyrroline-2-carboxylic acid	L-Glutamate 5-semialdehyde	
2-Oxo-4-hydroxy-5-aminovaleric		

Lysine Metabolism (28 Metabolites)

Lysine	Carnitine	6-Acetamido-2-Oxohexanoic Acid
(2R,3R)-3-Methylglutamyl-5-Semialdehyde-N6-Lysine	N-Alpha-Acetyllysine	6-Amino-2-Oxohexanoic Acid
(2R,3R)-3-Methylornithine	N6-Acetyl-Lysine	D-Lysopine
2-Amino-6-Oxoheptanedioic Acid	(3S,5S)-3,5-Diaminohexanoic acid	Delta1-Piperideine-2-Carboxylic Acid
Meso-2,6-Diaminoheptanedioic Acid	(S)-2,3,4,5-Tetrahydropyridine-2-Carboxylic Acid	N-Acetyl-Cadaverine
5-Aminopentanoic acid	(S)-5-Amino-3-oxohexanoic acid	N-Acetyl-L-2-Aminoadipic acid
5-Hydroxylysine	2-Amino-5-Oxohexanoic Acid	N-Acetyl-Pipecolic Acid
Aminoadipic acid	2-Aminoadipate 6-Semialdehyde	N6-(L-1,3-Dicarboxypropyl)-L-lysine
Cadaverine	5-Acetamidopentanoic Acid	N6-Hydroxy-L-lysine
	5-Oxopentanoic acid	

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Cysteine and Methionine Metabolism (24 Metabolites)

2-Aminobutyric acid	3-Sulfino-L-alanine	N-Acetyl-L-Cystine
3-(Methylthio) propionic acid	Dehydroalanine	N-Acetyl-Ophthalmic Acid
Cystine	Gamma-L-Glutamyl-L-2-Aminobutyric Acid	N-Formylmethionine
Homocystine	L-Cysteic acid	O-Acetyl-Homoserine
Methionine	L-Homocysteine	Ophthalmic acid
Methionine Sulfoxide	N-Acetyl-(S)-2-Aminobutanoic acid	S-Glutathionyl-L-cysteine
O-Acetyl-L-serine hydrochloride	N-Acetyl-Dehydroalanine	Thiocysteine
1-Aminocyclopropane-1-carboxylic acid	N-Acetyl-Gamma-Glutamyl-2-Aminobutyric Acid	
3-Mercaptolactic Acid		

Histidine Metabolism (19 Metabolites)

1-Methylhistidine	Imidazolepropionic Acid	Methylimidazoleacetic acid
3-Methylhistidine	Imidazolepyruvic Acid	N-Acetyl-N(pi)-Methyl-L-histidine
Acetyl-Histidine	Urocanic acid	N-Formimino-L-aspartic acid
Histamine	4-Oxoglutaramic acid	N-Formimino-L-glutamic acid
Histidine	Hydantoin-5-propionic acid	N-Formyl-L-aspartic acid
Histidinol	Isoglutamine	
Imidazoleacetic Acid	L-Histidinal	

Benzoate Metabolism (16 Metabolites)

Cyclohexane-1-Carboxylic Acid	4-Chlorobenzoic Acid	4-Aminocatechol
Resorcinol	4-Aminophenol	Cyclopropanecarboxylic Acid
2-Hydroxymuconic Acid	4-Nitrophenol	Mandelic Acid
3-Hydroxy-Cis,Cis-Muconic Acid	Guaiacol	O-Hydroxylaminobenzoic Acid
3-Oxoadipic Acid	Vanillic acid	
3-Fluoro-Cis,Cis-Muconic Acid	3-O-Methylgallic acid	