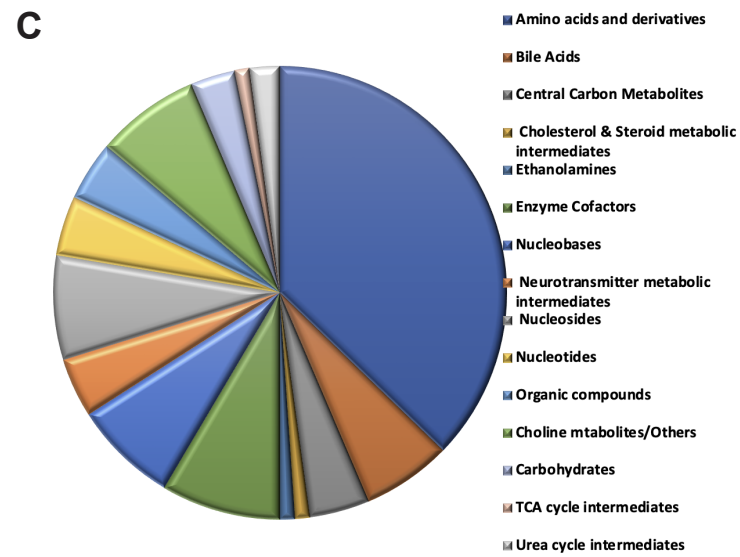


A

List of metabolites analyzed
Glycine
Trimethylamine-N-Oxide
Alanine
Glyceraldehyde
Aminoisobutyric acid
Dimethyl Glycine
GABA
Choline
Serine
Cytosine
Creatinine
Proline
Betaine
Valine
Guanidinoacetic Acid
Niacinamide (B3)
Taurine
1-methylhistamine
Isoleucine
Hydroxyproline
Asparagine
Ornithine
Leucine
Creatine
Aspartate
Adenine
3-OH-Anthranilic Acid
Homocysteine
Hypoxanthine
Phosphoethanolamine
Spermidine
Lysine
Glutamine
Glutamic Acid
Methionine
Histidine
Carnitine
Normetamphetamine
Phenylalanine
Pyridoxine (B6)
Arginine
Citrulline
Cotinine
Hippuric acid
Tyrosine
4-Pyridoxic Acid (B6)
Kynurenic Acid
5-Hydroxyindole-3-acetic acid
SDMA
Tryptophan
Kynurenine
Pantothenic Acid (B5)
L-5-Hydroxytryptophan
Cystathionine
3-OH-DL-KYNURENINE
Z-deoxycytidine
Cytidine
Carnosine
Neopterin
Adenosine
Xanthosine
Glutathione (reduced)
cAMP
AMP
Folic Acid (B9)
NAD
Acetoacetic acid
Uracil
Succinate
Homoserine
Threonine
Nicotinic Acid (B3)
Xanthine
Orotic acid
Alantoin
2-Aminodipic Acid
Homogentisic acid
Inositol (Bh?)
Sorbitol
Glucuronate
Z-deoxyuridine
Ribose-5-P
g-Glu-Cy(Gamma-Glutamylcysteine)
Inosine
Guanosine
Sucrose
cGMP
IMP
Chenodeoxycholic Acid
Cholic Acid
Glycocholic Acid
Taurchenodeoxycholic Acid
Taurocholic Acid
UDP-Glucose

B

Metabolite class	
Amino acids and derivatives	35
Bile Acids	6
Central Carbon Metabolites	4
Cholesterol & Steroid metabolic intermediates	1
Ethanolamines	1
Enzyme Cofactors	8
Nucleobases	7
Neurotransmitter metabolic intermediates	4
Nucleosides	7
Nucleotides	4
Organic compounds	4
Choline mtabolites/Others	7
Carbohydrates	3
TCA cycle intermediates	1
Urea cycle intermediates	2



D

List of metabolites that passed quality control
Glycine
Trimethylamine-N-Oxide
Alanine
Glyceraldehyde
Aminoisobutyric acid
Dimethyl Glycine
GABA
Choline
Serine
Cytosine
Creatinine
Proline
Betaine
Valine
Guanidinoacetic Acid
Niacinamide (B3)
Taurine
1-methylhistamine
Isoleucine
Hydroxyproline
Asparagine
Ornithine
Leucine
Creatine
Aspartate
Adenine
3-OH-Anthranilic Acid
Hypoxanthine
Phosphoethanolamine
Spermidine
Lysine
Glutamine
Glutamic Acid
Methionine
Histidine
Carnitine
Normetamphetamine
Phenylalanine
Arginine
Citrulline
Cotinine
Hippuric acid
Tyrosine
4-Pyridoxic Acid (B6)
Kynurenic Acid
SDMA
Tryptophan
Kynurenine
Pantothenic Acid (B5)
Cystathionine
Cytidine
Carnosine
Neopterin
Adenosine
Xanthosine
Glutathione (reduced)
cAMP
NAD
Uracil
Succinate
Homoserine
Threonine
Xanthine
Alantoin
2-Aminodipic Acid
Inositol (Bh?)
Sorbitol
Glucuronate
Z-deoxyuridine
Ribose-5-P
Inosine
Guanosine
Sucrose
IMP
Chenodeoxycholic Acid
Cholic Acid
Glycocholic Acid

Figure S1