

Supplementary Document S1.

Detailed chemical vendor information

Chemical standards including asymmetric dimethylarginine (ADMA), carnosine, creatinine, levodopa (DOPA), dopamine, histamine, trans-hydroxyproline, phenylethylamine, putrescine, sarcosine, serotonin, spermidine, spermine, taurine, tyramine, alanine, arginine, asparagine, aspartic acid, citrulline, glutamine, glutamic acid, glycine, histidine, leucine, isoleucine, lysine, methionine, ornithine, phenylalanine, proline, serine, threonine, tryptophan, valine, 3-methylhistidine, betaine, trimethylamine N-oxide (TMAO), choline, nitro-tyrosine, tyrosine, kynurenine, creatine, homoserine, zeatin, shikimic acid, glyceric acid, lactic acid, beta-hydroxybutyric acid, alpha-ketoglutaric acid, citric acid, butyric acid, propionic acid, succinic acid, fumaric acid, pyruvic acid, hippuric acid, methylmalonic acid, 5-hydroxyindoleacetic acid, para-hydroxyphenylacetic acid, malic acid, glutaric acid, valeric acid, benzoic acid, oxalic acid, oxaloacetic acid, salicylic acid, abscisic acid, trans-aconitic acid, jasmonic acid, indole-3-acetic acid, L-carnitine inner salt, acetyl-L-carnitine hydrochloride, propionyl-L-carnitine, butyryl-L-carnitine, hexanoyl-L-carnitine, octanoyl-L-carnitine, decanoyl-L-carnitine, dodecanoyl-L-carnitine, tetradecanoyl-L-carnitine, hexadecanoyl-L-carnitine, octadecanoyl-L-carnitine, N-stearoyl-D-erythro-sphingosylphosphorylcholine, 1,2-dilinolenoyl-sn-glycero-3-phosphocholine, 1,2-Dioctadecanoyl-sn-glycero-3-phosphocholine, 1-oleoyl-2-hydroxy-sn-glycero-3-phosphocholine, and glucose were all bought from Sigma-Aldrich (Oakville, CA). N₁, N₁₂-diacetylspermine hydrochloride and proline-betaine were purchased from Cayman Chemical (Ann Arbor, MI, U.S.A.). Other stable isotope (D, ¹³C, ¹⁵N)-labelled internal standards (ISTD) including D₂-ornithine, ¹⁵N-histidine, D₃-creatinine, D₃-DOPA, D₄-dopamine, ¹³C-tyrosine, ¹³C-D₃-methionine, D₃-proline, D₄-serotonin, D₄-putrescine, D₃-sarcosine, ¹³C₂-taurine, D₄-tyramine, ¹⁵N-alanine, ¹³C₆-arginine, ¹⁵N-asparagine, D₃-aspartic acid, D₇-citrulline, D₃-glutamic acid, D₅-glutamine, ¹³C₂-glycine, ¹³C-leucine, ¹⁵N-phenylalanine, ¹³C-serine, D₂-

threonine, $^{15}\text{N}_2$ -tryptophan, D₈-valine, D₉-TMAO and $^{15}\text{N}_2$ -uric acid were bought from Cambridge Isotope Laboratories Inc. (Tewksbury, MA, U.S.A.). D₈-spermine tetrahydrochloride, D₈-spermidine trihydrochloride were purchased from IsoSciences (Ambler, U.S.A.). D₆-N₁, N₁₂-diacetylspermine dihydrochloride and D₆-ADMA were bought from Toronto Research Chemicals (North York, CA). D₃-creatinine, D₉-choline chloride, D₉-betaine hydrochloride, 2-D₁-sodium L-lactate, D₄-sodium beta-hydroxybutyrate, 1- ^{13}C -alpha-ketoglutaric acid, D₄-citric acid, 1- ^{13}C -butyric acid, 1- ^{13}C -propionic acid, D₄-succinic acid, $^{13}\text{C}_2$ -D₂-fumaric acid, ^{13}C -pyruvic acid, D₂-hippuric acid, methyl-D₃-malonic acid, and D₂-indole-3-acetic acid were purchased from C/D/N Isotopes Inc. (Pointe-Claire, CA). Labelled carnitine standard set was purchased from Cambridge Isotope Laboratories Inc. (Tewksbury, U.S.A.). 1,2-dimyristoyl-sn-glycero-3-phosphocholine, 1,2-diarachidoyl-sn-glycero-3-phosphocholine, 1-nonanoyl-2-hydroxy-sn-glycero-3-phosphocholine, N-hexanoyl-D-erythro-sphingosylphosphorylcholine, and $^{13}\text{C}_6$ -glucose were bought from Sigma-Aldrich (Oakville, CA).