

## 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). N<sub>1</sub>, N<sub>12</sub>-diacetylspermine hydrochloride and proline-betaine were purchased from Cayman Chemical (Ann Arbor, MI, U.S.A.). Other stable isotope (D, <sup>13</sup>C, <sup>15</sup>N)-labelled internal standards (ISTD) including D<sub>2</sub>-ornithine, <sup>15</sup>N-histidine, D<sub>3</sub>-creatinine, D<sub>3</sub>-DOPA, D<sub>4</sub>-dopamine, <sup>13</sup>C-tyrosine, <sup>13</sup>C-D<sub>3</sub>-methionine, D<sub>3</sub>-proline, D<sub>4</sub>-serotonin, D<sub>4</sub>-putrescine, D<sub>3</sub>-sarcosine, <sup>13</sup>C<sub>2</sub>-taurine, D<sub>4</sub>-tyramine, <sup>15</sup>N-alanine, <sup>13</sup>C<sub>6</sub>-arginine, <sup>15</sup>N-asparagine, D<sub>3</sub>-aspartic acid, D<sub>7</sub>-citrulline, D<sub>3</sub>-glutamic acid, D<sub>5</sub>-glutamine, <sup>13</sup>C<sub>2</sub>-glycine, <sup>13</sup>C-leucine, <sup>15</sup>N-phenylalanine, <sup>13</sup>C-serine, D<sub>2</sub>-

threonine,  $^{15}\text{N}_2$ -tryptophan,  $\text{D}_8$ -valine,  $\text{D}_9$ -TMAO and  $^{15}\text{N}_2$ -uric acid were bought from Cambridge Isotope Laboratories Inc. (Tewksbury, MA, U.S.A.).  $\text{D}_8$ -spermine tetrahydrochloride,  $\text{D}_8$ -spermidine trihydrochloride were purchased from IsoSciences (Ambler, U.S.A.).  $\text{D}_6$ - $\text{N}_1$ ,  $\text{N}_{12}$ -diacetylspermine dihydrochloride and  $\text{D}_6$ -ADMA were bought from Toronto Research Chemicals (North York, CA).  $\text{D}_3$ -creatinine,  $\text{D}_9$ -choline chloride,  $\text{D}_9$ -betaine hydrochloride,  $2\text{-D}_1$ -sodium L-lactate,  $\text{D}_4$ -sodium beta-hydroxybutyrate,  $1\text{-}^{13}\text{C}$ -alpha-ketoglutaric acid,  $\text{D}_4$ -citric acid,  $1\text{-}^{13}\text{C}$ -butyric acid,  $1\text{-}^{13}\text{C}$ -propionic acid,  $\text{D}_4$ -succinic acid,  $^{13}\text{C}_2\text{-D}_2$ -fumaric acid,  $^{13}\text{C}$ -pyruvic acid,  $\text{D}_2$ -hippuric acid, methyl- $\text{D}_3$ -malonic acid, and  $\text{D}_2$ -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).