Supplementary Table S1 Coefficient of Variations (CV%) computed as defined in Material and methods. Metabolites with a CV% > 20% were excluded from the analysis.

|  |  |  |  |
| --- | --- | --- | --- |
| Metabolite class | Abbreviation1 | Biochemical Name2 | CV(%)  |
| Acylcarnitines | C0 | Carnitine | 8.3 |
|  | C10 | Decanoylcarnitine | 9.4 |
|  | C10:1 | Decenoylcarnitine | 55.8 |
|  | C10:2 | Decadienylcarnitine | 10.3 |
|  | C12 | Dodecanoylcarnitine | 11.6 |
|  | C12-DC | Dodecanedioylcarnitine | 14.3 |
|  | C12:1 | Dodecenoylcarnitine | 47.1 |
|  | C14 | Tetradecanoylcarnitine | 6.7 |
|  | C14:1 | Tetradecenoylcarnitine | 12.9 |
|  | C14:1-OH | Hydroxytetradecenoylcarnitine | 8.3 |
|  | C14:2 | Tetradecadienylcarnitine | 10.9 |
|  | C14:2-OH | Hydroxytetradecadienylcarnitine | 28.3 |
|  | C16 | Hexadecanoylcarnitine | 2.7 |
|  | C16-OH | Hydroxyhexadecanoylcarnitine | 15.7 |
|  | C16:1 | Hexadecenoylcarnitine | 5.7 |
|  | C16:1-OH | Hydroxyhexadecenoylcarnitine | 23.6 |
|  | C16:2 | Hexadecadienylcarnitine | 47.1 |
|  | C16:2-OH | Hydroxyhexadecadienylcarnitine | 10.9 |
|  | C18 | Octadecanoylcarnitine | 0.0 |
|  | C18:1 | Octadecenoylcarnitine | 3.3 |
|  | C18:1-OH | Hydroxyoctadecenoylcarnitine | 25.0 |
|  | C18:2 | Octadecadienylcarnitine | 15.7 |
|  | C2 | Acetylcarnitine | 7.6 |
|  | C3 | Propionylcarnitine | 14.8 |
|  | C3-DC (C4-OH) | Hydroxybutyrylcarnitine | 0.0 |
|  | C3-OH | Hydroxypropionylcarnitine | 3.8 |
|  | C3:1 | Propenonylcarnitine | 0.0 |
|  | C4 | Butyrylcarnitine | 5.8 |
|  | C4:1 | Butenylcarnitine | 2.0 |
|  | C5 | Valerylcarnitine | 14.1 |
|  | C5-DC (C6-OH) | Glutarylcarnitine | 11.8 |
|  | C5-M-DC | Methylglutarylcarnitine | 4.7 |
|  | C5-OH (C3-DC-M) | Hydroxyvalerylcarnitine (Methylmalonylcarnitine) | 3.4 |
|  | C5:1 | Tiglylcarnitine | 11.5 |
|  | C5:1-DC | Glutaconylcarnitine | 20.2 |
|  | C6 (C4:1-DC) | Hexanoylcarnitine | 0.0 |
|  | C6:1 | Hexenoylcarnitine | 9.4 |
|  | C7-DC | Pimelylcarnitine | 26.5 |
|  | C8 | Octanoylcarnitine | 0.0 |
|  | C9 | Nonaylcarnitine | 3.1 |
| Amino acids | Ala | Alanine | 2.8 |
|  | Arg | Arginine | 10.0 |
|  | Asn | Asparagine | 2.6 |
|  | Asp | Aspartate | NA |
|  | Cit | Citrulline | 5.7 |
|  | Gln | Glutamine | 15.8 |
|  | Glu | Glutamate | 3.5 |
|  | Gly | Glycine | 14.1 |
|  | His | Histidine | 12.5 |
|  | Ile | Isoleucine | 11.7 |
|  | Leu | Leucine | 10.8 |
|  | Lys | Lysine | 9.7 |
|  | Met | Methionine | 8.1 |
|  | Orn | Ornithine | 15.0 |
|  | Phe | Phenylalanine | 8.4 |
|  | Pro | Proline | 11.6 |
|  | Ser | Serine | 18.8 |
|  | Thr | Threonine | 8.6 |
|  | Trp | Tryptophan | 11.7 |
|  | Tyr | Tyrosine | 7.6 |
|  | Val | Valine | 7.5 |
| Biogenic amines | ADMA | Asymmetric dimethylarginine | 20.9 |
|  | Ac-Orn | Acetylornithine | 0.4 |
|  | Carnosine | Carnosine | 10.0 |
|  | Creatinine | Creatinine | 1.8 |
|  | Histamine | Histamine | NA |
|  | Kynurenine | Kynurenine | 5.0 |
|  | Met-SO | Methioninesulfoxide | 5.9 |
|  | Nitro-Tyr | Nitrotyrosine | NA |
|  | OH-Pro | Hydroxyproline | NA |
|  | PEA | Phenylethylamine | NA |
|  | Putrescine | Putrescine | 0.6 |
|  | SDMA | Symmetric Dimethylarginine | NA |
|  | Sarcosine | Sarcosine | 12.5 |
|  | Serotonin | Serotonin | 7.2 |
|  | Spermidine | Spermidine | 4.8 |
|  | Spermine | Spermine | 3.1 |
|  | Taurine | Taurine | 3.3 |
|  | alpha-AAA |  alpha-Aminoadipic acid | 15.0 |
|  | Total-DMA | Sum of ADMA and SDMA  | 13.1 |
| Phosphatidylcholine diacyl | PC aa C24:0 | Phosphatidylcholine diacyl C24:0 | 31.2 |
|  | PC aa C26:0 | Phosphatidylcholine diacyl C26:0 | 31.1 |
|  | PC aa C28:1 | Phosphatidylcholine diacyl C28:1 | 5.9 |
|  | PC aa C30:0 | Phosphatidylcholine diacyl C30:0 | 1.7 |
|  | PC aa C30:2 | Phosphatidylcholine diacyl C30:2 | 45.0 |
|  | PC aa C32:0 | Phosphatidylcholine diacyl C32:0 | 2.7 |
|  | PC aa C32:1 | Phosphatidylcholine diacyl C32:1 | 1.2 |
|  | PC aa C32:2 | Phosphatidylcholine diacyl C32:2 | 1.3 |
|  | PC aa C32:3 | Phosphatidylcholine diacyl C32:3 | 10.9 |
|  | PC aa C34:1 | Phosphatidylcholine diacyl C34:1 | 7.0 |
|  | PC aa C34:2 | Phosphatidylcholine diacyl C34:2 | 0.7 |
|  | PC aa C34:3 | Phosphatidylcholine diacyl C34:3 | 10.0 |
|  | PC aa C34:4 | Phosphatidylcholine diacyl C34:4 | 1.0 |
|  | PC aa C36:0 | Phosphatidylcholine diacyl C36:0 | 38.2 |
|  | PC aa C36:1 | Phosphatidylcholine diacyl C36:1 | 4.4 |
|  | PC aa C36:2 | Phosphatidylcholine diacyl C36:2 | 3.9 |
|  | PC aa C36:3 | Phosphatidylcholine diacyl C36:3 | 0.2 |
|  | PC aa C36:4 | Phosphatidylcholine diacyl C36:4 | 2.5 |
|  | PC aa C36:5 | Phosphatidylcholine diacyl C36:5 | 5.1 |
|  | PC aa C36:6 | Phosphatidylcholine diacyl C36:6 | 7.5 |
|  | PC aa C38:0 | Phosphatidylcholine diacyl C38:0 | 5.0 |
|  | PC aa C38:1 | Phosphatidylcholine diacyl C38:1 | 35.5 |
|  | PC aa C38:3 | Phosphatidylcholine diacyl C38:3 | 2.7 |
|  | PC aa C38:4 | Phosphatidylcholine diacyl C38:4 | 5.2 |
|  | PC aa C38:5 | Phosphatidylcholine diacyl C38:5 | 3.2 |
|  | PC aa C38:6 | Phosphatidylcholine diacyl C38:6 | 1.0 |
|  | PC aa C40:1 | Phosphatidylcholine diacyl C40:1 | 11.3 |
|  | PC aa C40:2 | Phosphatidylcholine diacyl C40:2 | 0.1 |
|  | PC aa C40:3 | Phosphatidylcholine diacyl C40:3 | 11.9 |
|  | PC aa C40:4 | Phosphatidylcholine diacyl C40:4 | 2.3 |
|  | PC aa C40:5 | Phosphatidylcholine diacyl C40:5 | 6.4 |
|  | PC aa C40:6 | Phosphatidylcholine diacyl C40:6 | 0.0 |
|  | PC aa C42:0 | Phosphatidylcholine diacyl C42:0 | 0.7 |
|  | PC aa C42:1 | Phosphatidylcholine diacyl C42:1 | 14.8 |
|  | PC aa C42:2 | Phosphatidylcholine diacyl C42:2 | 0.5 |
|  | PC aa C42:4 | Phosphatidylcholine diacyl C42:4 | 5.2 |
|  | PC aa C42:5 | Phosphatidylcholine diacyl C42:5 | 6.8 |
|  | PC aa C42:6 | Phosphatidylcholine diacyl C42:6 | 5.4 |
| Phosphatidylcholine acyl-akyl | PC ae C30:0 | Phosphatidylcholine acyl-akyl C30:0 | 4.3 |
|  | PC ae C30:1 | Phosphatidylcholine acyl-akyl C30:1 | 23.7 |
|  | PC ae C30:2 | Phosphatidylcholine acyl-akyl C30:2 | 32.4 |
|  | PC ae C32:1 | Phosphatidylcholine acyl-akyl C32:1 | 8.1 |
|  | PC ae C32:2 | Phosphatidylcholine acyl-akyl C32:2 | 22.0 |
|  | PC ae C34:0 | Phosphatidylcholine acyl-akyl C34:0 | 9.7 |
|  | PC ae C34:1 | Phosphatidylcholine acyl-akyl C34:1 | 6.6 |
|  | PC ae C34:2 | Phosphatidylcholine acyl-akyl C34:2 | 2.0 |
|  | PC ae C34:3 | Phosphatidylcholine acyl-akyl C34:3 | 3.0 |
|  | PC ae C36:0 | Phosphatidylcholine acyl-akyl C36:0 | 21.6 |
|  | PC ae C36:1 | Phosphatidylcholine acyl-akyl C36:1 | 7.7 |
|  | PC ae C36:2 | Phosphatidylcholine acyl-akyl C36:2 | 3.3 |
|  | PC ae C36:3 | Phosphatidylcholine acyl-akyl C36:3 | 8.7 |
|  | PC ae C36:4 | Phosphatidylcholine acyl-akyl C36:4 | 6.7 |
|  | PC ae C36:5 | Phosphatidylcholine acyl-akyl C36:5 | 0.4 |
|  | PC ae C38:0 | Phosphatidylcholine acyl-akyl C38:0 | 0.1 |
|  | PC ae C38:1 | Phosphatidylcholine acyl-akyl C38:1 | 11.4 |
|  | PC ae C38:2 | Phosphatidylcholine acyl-akyl C38:2 | 5.7 |
|  | PC ae C38:3 | Phosphatidylcholine acyl-akyl C38:3 | 0.9 |
|  | PC ae C38:4 | Phosphatidylcholine acyl-akyl C38:4 | 4.5 |
|  | PC ae C38:5 | Phosphatidylcholine acyl-akyl C38:5 | 6.6 |
|  | PC ae C38:6 | Phosphatidylcholine acyl-akyl C38:6 | 2.8 |
|  | PC ae C40:1 | Phosphatidylcholine acyl-akyl C40:1 | 3.8 |
|  | PC ae C40:2 | Phosphatidylcholine acyl-akyl C40:2 | 5.2 |
|  | PC ae C40:3 | Phosphatidylcholine acyl-akyl C40:3 | 1.1 |
|  | PC ae C40:4 | Phosphatidylcholine acyl-akyl C40:4 | 1.1 |
|  | PC ae C40:5 | Phosphatidylcholine acyl-akyl C40:5 | 7.4 |
|  | PC ae C40:6 | Phosphatidylcholine acyl-akyl C40:6 | 7.2 |
|  | PC ae C42:0 | Phosphatidylcholine acyl-akyl C42:0 | 8.0 |
|  | PC ae C42:1 | Phosphatidylcholine acyl-akyl C42:1 | 17.7 |
|  | PC ae C42:2 | Phosphatidylcholine acyl-akyl C42:2 | 6.0 |
|  | PC ae C42:3 | Phosphatidylcholine acyl-akyl C42:3 | 15.9 |
|  | PC ae C42:4 | Phosphatidylcholine acyl-akyl C42:4 | 1.1 |
|  | PC ae C42:5 | Phosphatidylcholine acyl-akyl C42:5 | 0.0 |
|  | PC ae C44:3 | Phosphatidylcholine acyl-akyl C44:3 | 21.6 |
|  | PC ae C44:4 | Phosphatidylcholine acyl-akyl C44:4 | 7.7 |
|  | PC ae C44:5 | Phosphatidylcholine acyl-akyl C44:5 | 16.6 |
|  | PC ae C44:6 | Phosphatidylcholine acyl-akyl C44:6 | 1.3 |
|  | lysoPC a C14:0 | lysoPhosphatidylcholine acyl C14:0 | 2.8 |
|  | lysoPC a C16:0 | lysoPhosphatidylcholine acyl C16:0 | 5.6 |
| lysoPhosphatidylcholine acyl | lysoPC a C16:1 | lysoPhosphatidylcholine acyl C16:1 | 5.4 |
|  | lysoPC a C17:0 | lysoPhosphatidylcholine acyl C17:0 | 8.3 |
|  | lysoPC a C18:0 | lysoPhosphatidylcholine acyl C18:0 | 10.5 |
|  | lysoPC a C18:1 | lysoPhosphatidylcholine acyl C18:1 | 8.7 |
|  | lysoPC a C18:2 | lysoPhosphatidylcholine acyl C18:2 | 2.2 |
|  | lysoPC a C20:3 | lysoPhosphatidylcholine acyl C20:3 | 5.8 |
|  | lysoPC a C20:4 | lysoPhosphatidylcholine acyl C20:4 | 7.2 |
|  | lysoPC a C24:0 | lysoPhosphatidylcholine acyl C24:0 | 33.0 |
|  | lysoPC a C26:0 | lysoPhosphatidylcholine acyl C26:0 | 23.6 |
|  | lysoPC a C26:1 | lysoPhosphatidylcholine acyl C26:1 | 3.9 |
|  | lysoPC a C28:0 | lysoPhosphatidylcholine acyl C28:0 | 28.4 |
|  | lysoPC a C28:1 | lysoPhosphatidylcholine acyl C28:1 | 28.7 |
| Sphingomyelins | SM (OH) C14:1 | Hydroxysphingomyeline C14:1 | 1.7 |
|  | SM (OH) C16:1 | Hydroxysphingomyeline C16:1 | 0.3 |
|  | SM (OH) C22:1 | Hydroxysphingomyeline C22:1 | 4.3 |
|  | SM (OH) C22:2 | Hydroxysphingomyeline C22:2 | 3.4 |
|  | SM (OH) C24:1 | Hydroxysphingomyeline C24:1 | 4.5 |
|  | SM C16:0 | Sphingomyeline C16:0 | 0.5 |
|  | SM C16:1 | Sphingomyeline C16:1 | 1.9 |
|  | SM C18:0 | Sphingomyeline C18:0 | 5.2 |
|  | SM C18:1 | Sphingomyeline C18:1 | 7.3 |
|  | SM C20:2 | Sphingomyeline C20:2 | 9.8 |
|  | SM C22:3 | Sphingomyeline C22:3 | 141.4 |
|  | SM C24:0 | Sphingomyeline C24:0 | 1.9 |
|  | SM C24:1 | Sphingomyeline C24:1 | 8.1 |
|  | SM C26:0 | Sphingomyeline C26:0 | 141.4 |
|  | SM C26:1 | Sphingomyeline C26:1 | 51.2 |
| Hexoses | H1 | Hexose | 4.9 |

1Abbreviations provided by Biocrates.

2Complete biochemical name of metabolites following the IUPAC nomenclature.