# Supplementary Figures and Tables

# Determinants of the urinary and serum metabolome in children from six European populations

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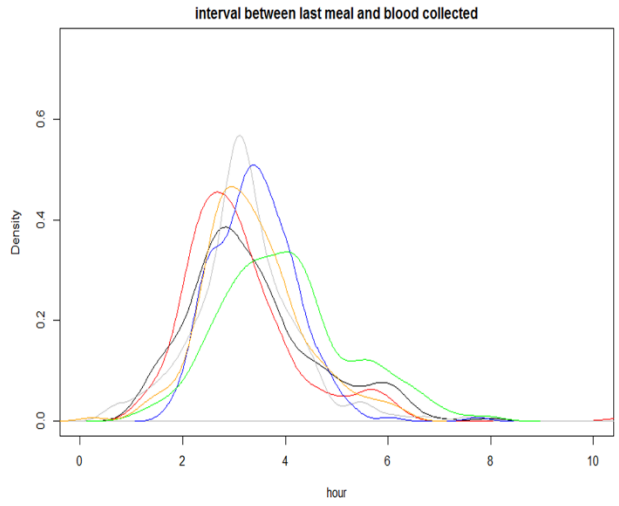
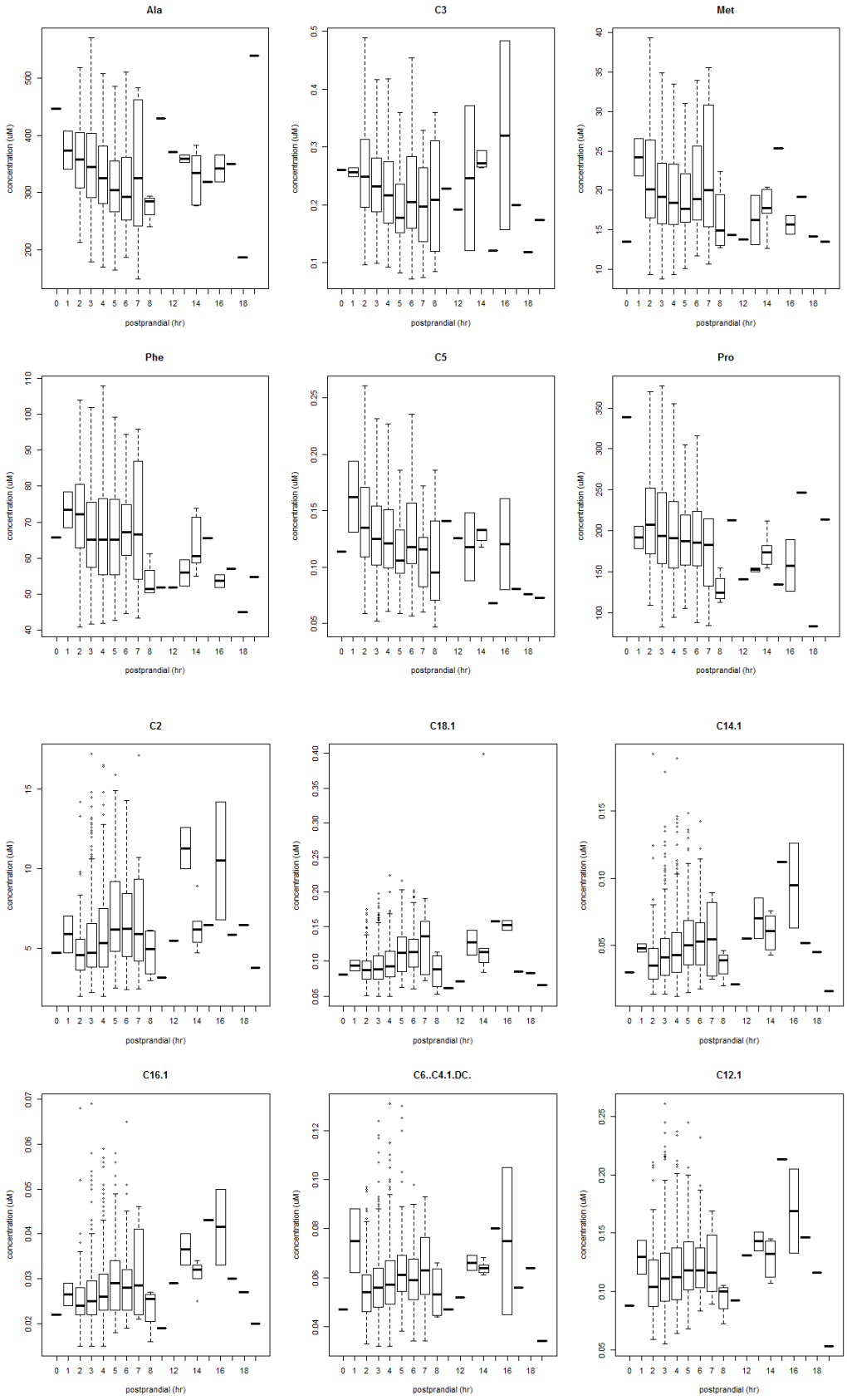
**Supplementary Figure 1 Distribution of postprandial time interval (between last meal and blood sample collection)**

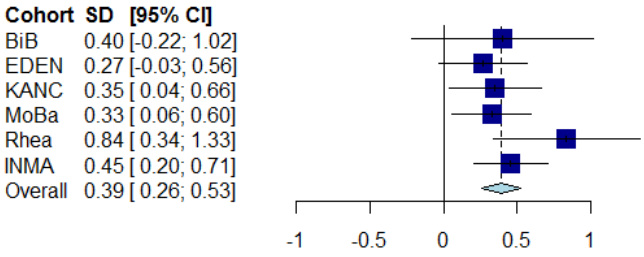



BiB; INMA; EDEN; MoBa; Rhea; KANC

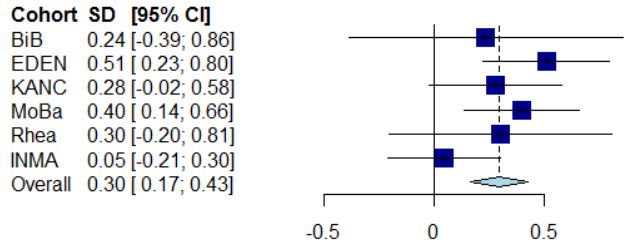
**Supplementary Figure 2 Effect of postprandial period on serum metabolite levels**



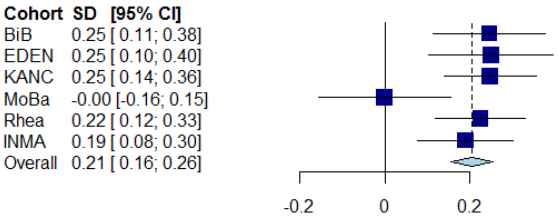
**Supplementary Figure 3 Associations between urine creatinine and age by cohort.** Coefficients represent SD per year



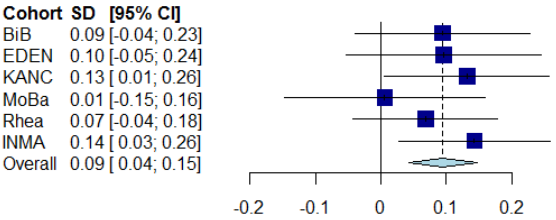

**Supplementary Figure 4 Associations between serum creatinine and age by cohort.** Coefficients represent SD per year



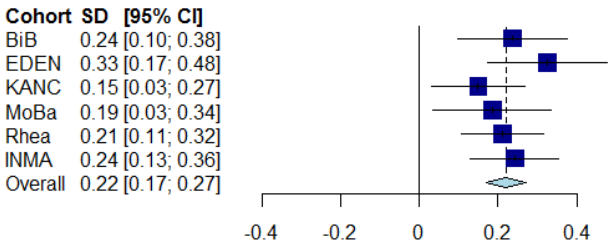

**Supplementary Figure 5 Associations of urine 4-deoxyerythronic acid with zBMI by cohort.** Coefficients represent SD per BMI z-score



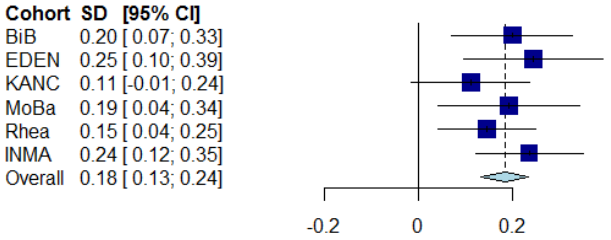

**Supplementary Figure 6 Associations of urine valine with zBMI by cohort.** Coefficients represent SD per BMI z-score



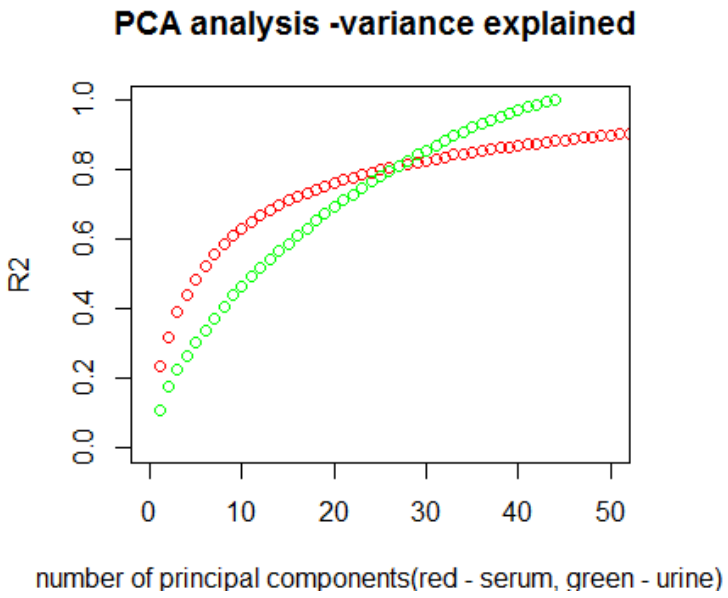
**Supplementary Figure 7 Associations of serum glutamate with zBMI by cohort.** Coefficients represent SD per BMI z-score



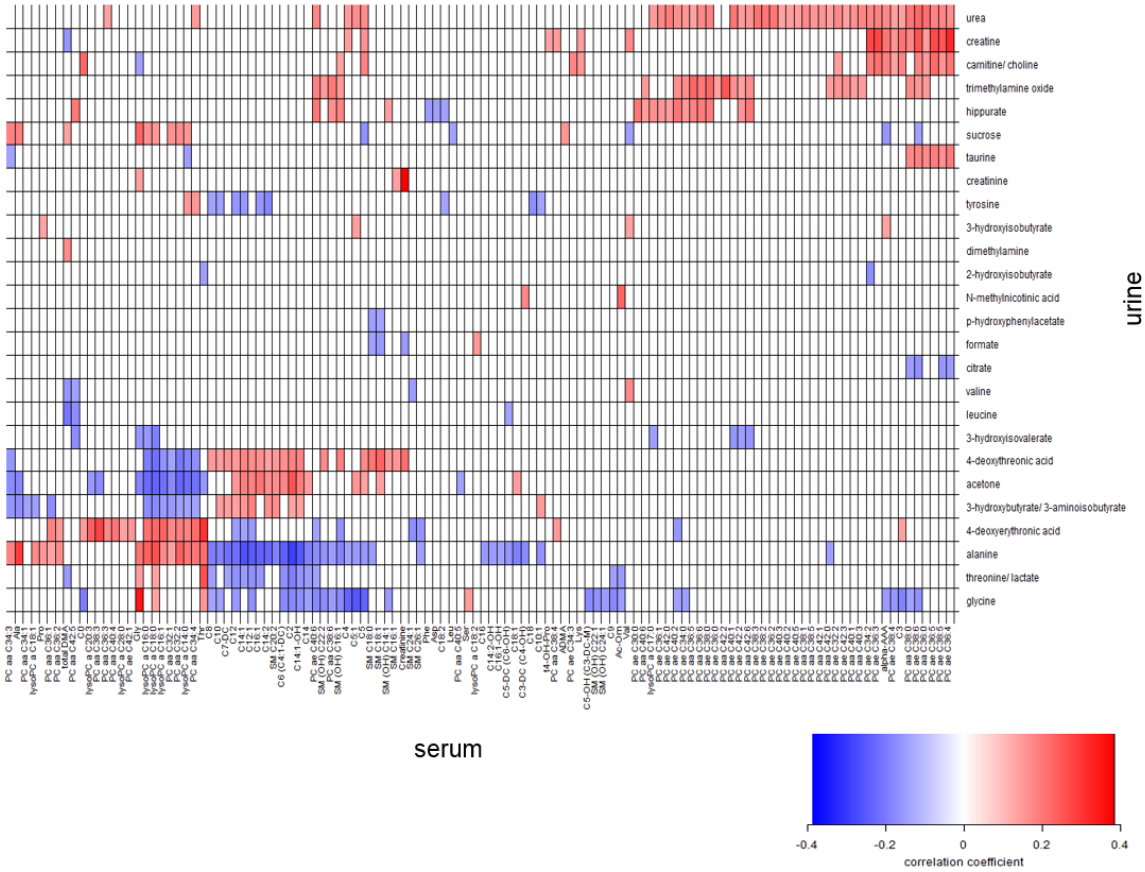

**Supplementary Figure 8 Associations of serum carnitine (C0) with zBMI by cohort**




**Supplementary Figure 9 PCA analysis - cumulative $R^2$ (variance explained) of the urine and serum data model.** Data were log10 transformed, mean-centred and univariate scaled prior to modelling



**Supplementary Figure 10 Cross urine-serum metabolic correlation based on pairwise correlations across the two bio fluid types.**



**Supplementary Table 1 $^{1}$H NMR spectroscopy urinary metabolite annotations and assignments**

| Metabolite | ChEBI ID | HMDB ID | Compound Class | Resonance (δ / ppm) | Evidence for assignment |
|---|---|---|---|---|---|
| leucine | 25017 | HMDB0000687 | Amino acids, peptides, and analogues | 0.97 | TOCSY |
| isoleucine | 24898 | HMDB0000172 | Amino acids, peptides, and analogues | 1.02 | TOCSY |
| valine | 27266 | HMDB0000883 | Amino acids, peptides, and analogues | 1.04 | TOCSY |
| 3-hydroxyisobutyrate | 11805 | HMDB0000023 | Beta hydroxy acids and derivatives | 1.08 | HSQC |
| 4-deoxyerythronic acid | 86347 | HMDB0000498 | Sugar acids and derivatives | 1.11 | TOCSY, Spike-in |
| 4-deoxythreonic acid | 86391 | HMDB0002453 | Sugar acids and derivatives | 1.24 | TOCSY, Spike-in |
| threonine / lactate | 26986/24996 | HMDB0000167/ HMDB0000190 | Amino acids, peptides, and analogues/ Alpha hydroxy acids and derivatives | 1.33 | STOCSY, HSQC |
| 2-hydroxyisobutyrate | 19641 | HMDB0000729 | Alpha hydroxy acids and derivatives | 1.36 | HSQC |
| alanine | 16977 | HMDB0000161 | Amino acids, peptides, and analogues | 1.48 | STOCSY |
| lysine | 25094 | HMDB0000182 | Amino acids, peptides, and analogues | 1.74 | STOCSY |
| acetate | 30089 | HMDB0000042 | Carboxylic acids | 1.93 | HSQC |
| *p*-cresol sulfate | 82914 | HMDB0011635 | Arylsulfates | 2.35 | HSQC, STOCSY |
| succinate | 26806 | HMDB0000254 | Dicarboxylic acids and derivatives | 2.41 | HSQC |
| glutamine | 28300 | HMDB0000641 | Amino acids, peptides, and analogues | 2.46 | STOCSY |
| citrate | 30769 | HMDB0000094 | Tricarboxylic acids and derivatives | 2.54 | STOCSY |
| dimethylamine | 17170 | HMDB0000087 | amines | 2.73 | STOCSY |
| trimethylamine | 18139 | HMDB0000906 | Amines | 2.87 | HSQC |
| carnitine / choline | 17126/15354 | HMDB0000062/ HMDB0000097 | Carnitines/ Cholines | 3.23 | HSQC |
| trimethylamine *N*-oxide | 15724 | HMDB0000925 | Aminoxides | 3.28 | HSQC |
| *scyllo*-inositol | 10642 | HMDB0006088 | Alcohols and polyols | 3.37 | HSQC |
| taurine | 15891 | HMDB0000251 | Organosulfonic acids | 3.43 | STOCSY |
| glycine | 15428 | HMDB0000123 | Amino acids, peptides, and analogues | 3.58 | HSQC |
| creatine | 16919 | HMDB0000064 | Amino acids, peptides, and analogues | 3.94 | HSQC |
| creatinine | 16737 | HMDB0000562 | Amino acids, peptides, and analogues | 4.06 | HSQC |
| hippurate | 132966 | HMDB0000714 | Benzoic acids and derivatives | 7.56 | STOCSY |
| formate | 15740 | HMDB0000142 | Carboxylic acids | 8.47 | HSQC |
| pantothenic acid | 7916 | HMDB0000210 | Polyols | 0.94 | Spike-in |
| 3-hydroxybutyrate / 3-aminoisobutyrate | 37054/49096 | HMDB0000357/HMDB0003911 | Beta hydroxy acids and derivatives/ Amino acids, peptides, and analogues | 1.19 | TOCSY, Spike-in |
| 3-hydroxyisovalerate | 82957 | HMDB0000754 | Hydroxy fatty acids | 1.27 | STOCSY |
| *N*-acetyl neuraminic acid | 45744 | HMDB0000230 | Carbohydrates and carbohydrate conjugates | 2.06 | Spike-in |
| acetone | 15347 | HMDB0001659 | Ketones | 2.24 | HSQC |
| 5-oxoproline | 16010 | HMDB0000267 | Amino acids, peptides, and analogues | 2.39 | TOCSY, HSQC, Spike-in |
| 3-aminoisobutyrate | 49096 | HMDB0003911 | Amino acids, peptides, and analogues | 2.62 | TOCSY |
| proline betaine | 35280 | HMDB0004827 | Amino acids, peptides, and analogues | 3.30 | HSQC |
| glucose | 17234 | HMDB0000122 | Carbohydrates and carbohydrate conjugates | 5.25 | TOCSY, HSQC, STOCSY |

| Metabolite | ChEBI ID | HMDB ID | Compound Class | Resonance (δ / ppm) | Evidence for assignment |
|---|---|---|---|---|---|
| sucrose | 17992 | HMDB0000258 | Carbohydrates and carbohydrate conjugates | 5.42 | TOCSY, HSQC, STOCSY |
| urea | 16199 | HMDB0000294 | Organic carbonic acids and derivatives | 5.81 | tentative |
| *N*-methyl-2-pyridone-5-carboxamide | 27410 | HMDB0004193 | Nicotinamides | 6.67 | TOCSY, STOCSY, Spike-in |
| *p*-hydroxyphenylacetate | 18101 | HMDB0000020 | Phenols | 6.88 | STOCSY |
| tyrosine | 18186 | HMDB0000158 | Amino acids, peptides, and analogues | 6.91 | TOCSY |
| 3-Indoxylsulfate | 43355 | HMDB0000682 | Arylsulfates | 7.52 | TOCSY, HSQC, STOCSY |
| *N*-methylpicolinic acid | 69061 | Not Available | Alkaloids and derivatives | 8.72 | TOCSY |
| *N*-methylnicotinic acid | 50521 | HMDB0000875 | Alkaloids and derivatives | 9.12 | STOCSY |
| $N_1$-methyl-nicotinamide | 16797 | HMDB0000699 | Nicotinamides | 9.28 | STOCSY |

NB. Assignments were ambiguous for 3 of the metabolite signals: Threonine / Lactate (δ 1.33) – resonance peak contain signal contributions from both threonine and lactate. Carnitine / Choline (δ 3.23) - resonance peak contain signal contributions from both carnitine and choline. 3-hydroxybutyrate / 3-aminoisobutyrate (δ 1.19) - resonance peak contain signal contributions from both 3-hydroxybutyrate and 3-aminoisobutyrate. HMDB identifier for *N*-methylpicolinic acid cannot be located on the Human Metabolome Database website.

**Supplementary Table 2 Non-detection rates of urinary metabolites and coefficient of variation (CV)**

| Signals | Non-detected (%) | Coefficient of variation (%) |
|---|---|---|
| creatinine | 0% | 7% |
| leucine | 0% | 7% |
| isoleucine | 1% | 14% |
| valine | 0% | 10% |
| 3-hydroxyisobutyrate | 0% | 7% |
| 4-deoxyerythronic acid | 0% | 8% |
| 4-deoxythreonic acid | 0% | 6% |
| threonine/ lactate | 0% | 4% |
| 2-hydroxyisobutyrate | 0% | 6% |
| alanine | 0% | 6% |
| lysine | 0% | 7% |
| acetate | 0% | 22% |
| *p*-cresol sulfate | 0% | 8% |
| succinate | 7% | 12% |
| glutamine | 1% | 5% |
| citrate | 0% | 7% |
| dimethylamine | 1% | 14% |
| trimethylamine | 0% | 7% |
| carnitine / choline | 1% | 12% |
| trimethylamine *N*-oxide | 2% | 6% |
| *scyllo*-inositol | 4% | 17% |
| taurine | 1% | 5% |
| glycine | 0% | 9% |
| creatine | 0% | 7% |
| hippurate | 0% | 6% |
| formate | 0% | 9% |
| pantothenic acid | 0% | 7% |
| 3-hydroxybutyrate / 3-aminoisobutyrate | 3% | 10% |
| 3-hydroxyisovalerate | 0% | 6% |
| *N*-acetyl neuraminic acid | 1% | 13% |
| acetone | 1% | 28% |
| 5-oxoproline | 1% | 12% |
| 3-aminoisobutyrate | 2% | 10% |
| proline betaine | 8% | 20% |
| glucose | 0% | 11% |
| sucrose | 1% | 6% |
| urea | 0% | 8% |
| *N*-methyl-2-pyridone-5-carboxamide | 6% | 12% |
| *p*-hydroxyphenylacetate | 0% | 7% |
| tyrosine | 0% | 10% |
| 3-Indoxylsulfate | 2% | 15% |
| *N*-methylpicolinic acid | 46% | 27% |
| *N*-methylnicotinic acid | 0% | 13% |
| $N_1$-methyl nicotinamide | 1% | 20% |

**Supplementary Table 3 Coefficient of variation (CV) and percentage of measurments below the limit of detection (%BLD) per metabolite**

| Metabolite short name | Common name | ChEBI ID | Class | Assay | CV % | % BLD |
|---|---|---|---|---|---|---|
| Ala | L-Alanine | 15570 / 16977 | aminoacids | LC | 7.5 | 0 |
| Arg | L-Arginine | 29016 / 15816 / 16467 | aminoacids | LC | 8.3 | 0 |
| Asn | L-Asparagine | 22653 / 17196 / 28159 | aminoacids | LC | 8.1 | 0 |
| Asp | L-Aspartic acid | 22660 / 17053 / 17364 | aminoacids | LC | 14.9 | 0 |
| Cit | L-Citrulline | 18211 / 16349 / 49007 | aminoacids | LC | 10.2 | 0 |
| Gln | L-Glutamine | 28300 / 17061 / 18050 | aminoacids | LC | 7.7 | 0 |
| Glu | L-Glutamic acid | 18237 / 15966 / 16015 | aminoacids | LC | 9 | 0 |
| Gly | Glycine | 15428 | aminoacids | LC | 7 | 0 |
| His | L-Histidine | 27570 / 15971 / 27947 | aminoacids | LC | 7.8 | 0 |
| Ile | L-Isoleucine | 38264 / 22359 / 24898 / 17191 / 43433 | aminoacids | LC | 7.6 | 0 |
| Leu | L-Leucine | 25017 / 15603 / 28225 | aminoacids | LC | 7.8 | 0 |
| Lys | L-Lysine | 25094 / 16855 / 18019 | aminoacids | LC | 9 | 0 |
| Met | L-Methionine | 16811 / 16643 / 16867 | aminoacids | LC | 12.2 | 0 |
| Orn | L-Ornithine | 18257 / 15729 / 16176 | aminoacids | LC | 8.6 | 0 |
| Phe | L-Phenylalanine | 28044 / 16998 / 17295 | aminoacids | LC | 8.4 | 0 |
| Pro | L-Proline | 26271 / 16313 / 17203 | aminoacids | LC | 7.9 | 0 |
| Ser | L-Serine | 17822 / 16523 / 17115 | aminoacids | LC | 8 | 0 |
| Thr | L-Threonine | 16857 / 38263 / 26986 / 28718 / 38262 | aminoacids | LC | 8 | 0 |
| Trp | L-Tryptophan | 27897 / 16296 / 16828 | aminoacids | LC | 8.5 | 0 |
| Tyr | L-Tyrosine | 18186 / 17895 / 28479 | aminoacids | LC | 8.4 | 0 |
| Val | L-Valine | 27266 / 16414 / 27477 | aminoacids | LC | 7.3 | 0 |
| Ac-Orn | N-Acetylornithine | 16543 / 44673 | biogenic amines | LC | 14.5 | 19.2 |
| ADMA | Asymmetric dimethylarginine | 17929 | biogenic amines | LC | 11.8 | 0 |
| alpha-AAA | alpha-Aminoadipic acid | 37024 / 37023 / 37025 | biogenic amines | LC | 21.8 | 5.6 |
| Creatinine | Creatinine | 16737 | biogenic amines | LC | 7.5 | 0 |
| Histamine (#) | Histamine | 18295 | biogenic amines | LC | 56.5 | 100 |
| Kynurenine | Kynurenine | 28683 / 16946 / 86262 | biogenic amines | LC | 9.6 | 0 |
| Met-SO | Methionine Sulfoxide | 17016 / 49031 / 49032 / 49033 / 49034 | biogenic amines | LC | 16.4 | 4.8 |
| Putrescine | Putrescine | 17148 | biogenic amines | LC | 44.8 | 5.1 |
| SDMA | Symmetric dimethylarginine | 25682 | biogenic amines | LC | 35.9 | 5.4 |
| Serotonin | Serotonin | 28790 | biogenic amines | LC | 24 | 0 |
| Spermidine | Spermidine | 16610 | biogenic amines | LC | 17.1 | 66.5 |
| Spermine | Spermine | 15746 | biogenic amines | LC | 36.6 | 3 |
| t4-OH-Pro | trans-4-Hydroxyproline | 18095 / 86499 / 20392 | biogenic amines | LC | 10 | 0 |
| Taurine | Taurine | 15891 | biogenic amines | LC | 7.6 | 0 |
| total DMA | Total dimethylarginine | 86468 / 17929 / 25682 | biogenic amines | LC | 14.1 | 0 |
| c4-OH-Pro (#) | cis-4-Hydroxyproline | 18095 / 20392 | biogenic amines | LC | NA | 99.9 |
| Carnosine (#) | Carnosine | 15727 | biogenic amines | LC | 274.9 | 97.9 |
| DOPA (#) | DOPA | 49168 / 49169 / 15765 | biogenic amines | LC | NA | 99.9 |
| Dopamine (#) | Dopamine | 18243 | biogenic amines | LC | 306.2 | 99.0 |
| Nitro-Tyr (#) | Nitrotyrosine | 86267 | biogenic amines | LC | 617.2 | 100.0 |
| PEA (#) | Phenylethylamine | 50048 | biogenic amines | LC | 612.3 | 97.7 |
| C0 | L-Carnitine | 17126 / 11060 / 16347 | acylcarnitines | FIA | 7.6 | 0 |

| Metabolite short name | Common name | ChEBI ID | Class | Assay | CV % | % BLD |
|---|---|---|---|---|---|---|
| C10 | Decanoylcarnitine | 68830 / 28717 | acylcarnitines | FIA | 8.6 | 16.9 |
| C10:1 | Decenoylcarnitine | 86063 / 73048 | acylcarnitines | FIA | 10.3 | 68.6 |
| C10:2 | Decadienylcarnitine | Not Available | acylcarnitines | FIA | 8.8 | 99.8 |
| C12 | Dodecanoylcarnitine | 73054 / 77086 | acylcarnitines | FIA | 8.1 | 82.5 |
| C12-DC | Dodecanedioylcarnitine | 74121 | acylcarnitines | FIA | 9.4 | 100 |
| C12:1 | Dodecenoylcarnitine | 89717 / 86065 / 73053 | acylcarnitines | FIA | 10.1 | 71.3 |
| C14 | Tetradecanoylcarnitine | 73061 / 84634 | acylcarnitines | FIA | 13.8 | 99.5 |
| C14:1 | Tetradecenoylcarnitine | 86066 / 83049 / 85449 | acylcarnitines | FIA | 11.9 | 1.2 |
| C14:1-OH | Hydroxytetradecenoylcarnitine | 86067 / 73062 | acylcarnitines | FIA | 13.4 | 98.8 |
| C14:2 | Tetradecadienylcarnitine | 86069 / 73059 / 85451 | acylcarnitines | FIA | 12.1 | 30.6 |
| C14:2-OH | Hydroxytetradecadienylcarnitine | 86070 / 73108 / 85453 | acylcarnitines | FIA | 19.2 | 100 |
| C16 | Hexadecanoylcarnitine | 73067 / 17490 | acylcarnitines | FIA | 10.4 | 0.1 |
| C16-OH | Hydroxyhexadecanoylcarnitine | 73070 / 86030 | acylcarnitines | FIA | 24 | 100 |
| C16:1 | Hexadecenoylcarnitine | 86032 / 86031 | acylcarnitines | FIA | 8.9 | 93.3 |
| C16:1-OH | Hydroxyhexadecenoylcarnitine | 86033 / 85456 | acylcarnitines | FIA | 14.4 | 98.5 |
| C16:2 | Hexadecadienylcarnitine | 86035 / 73065 | acylcarnitines | FIA | 22.5 | 99.4 |
| C16:2-OH | Hydroxyhexadecadienylcarnitine | 73109 / 86036 | acylcarnitines | FIA | 11.9 | 100 |
| C18 | Octadecanoylcarnitine | 84644 / 73074 | acylcarnitines | FIA | 10.1 | 10.3 |
| C18:1 | Octadecenoylcarnitine | 86475 / 72689 / 86038 | acylcarnitines | FIA | 9 | 30.9 |
| C18:1-OH (#) | Hydroxyoctadecenoylcarnitine | 86039 / 73076 | acylcarnitines | FIA | 56.7 | 100 |
| C18:2 | Octadecadienylcarnitine | 86480 / 72715 / 85463 | acylcarnitines | FIA | 10.6 | 1.5 |
| C2 | Acetylcarnitine | 73024 / 57589 / 86045 | acylcarnitines | FIA | 7.4 | 0 |
| C3 | Propionylcarnitine | 28867 / 53210 | acylcarnitines | FIA | 15.9 | 0 |
| C3-DC (C4-OH) | Hydroxybutyrylcarnitine | 86047 / 73028 / 72995 / 84842 | acylcarnitines | FIA | 17.4 | 67.2 |
| C3-OH | Hydroxypropionylcarnitine | 86072 | acylcarnitines | FIA | 29.4 | 99.9 |
| C3:1 (#) | Propenoylcarnitine | 86073 | acylcarnitines | FIA | 65.5 | 100 |
| C4 | Butyrylcarnitine | 7676 / 21949 / 73017 / 84838 / 84838 | acylcarnitines | FIA | 16.5 | 0 |
| C4:1 | Butenylcarnitine | 88785 | acylcarnitines | FIA | 15.4 | 99.7 |
| C6 (C4:1-DC) | Fumaryl-L-carnitine / Hexanoyl-L-carnitine | 70749 / 84834 / 87264 | acylcarnitines | FIA | 10.1 | 79.8 |
| C5 | Valeryl-L-carnitine | 86492 / 73025 / 70819 / 73026 / 86050 / 86049 | acylcarnitines | FIA | 9.4 | 1.4 |
| C5-M-DC | Methylglutarylcarnitine | 86486 / 70857 | acylcarnitines | FIA | 17.3 | 99.9 |
| C5-OH (C3-DC-M) | Hydroxyvalerylcarnitine (Methylmalonylcarnitine) | 86467 / 73031 | acylcarnitines | FIA | 8.7 | 100 |
| C5:1 | Tiglylcarnitine | 71179 / 85520 | acylcarnitines | FIA | 17.2 | 100 |
| C5:1-DC | Glutaconylcarnitine | 86081 / 85518 | acylcarnitines | FIA | 21.7 | 99.9 |
| C5-DC (C6-OH) | Glutaryl-L-carnitine / Hydroxyhexanoyl-L-carnitine | 73040 / 82952 / 88772 | acylcarnitines | FIA | 17.7 | 98.5 |
| C6:1 | Hexenoylcarnitine | 88762 / 86082 | acylcarnitines | FIA | 14.1 | 99.9 |
| C7-DC | Pimelylcarnitine | 86084 / 85525 | acylcarnitines | FIA | 13.5 | 99.7 |
| C8 | Octanoylcarnitine | 73039 / 18102 / 86051 | acylcarnitines | FIA | 10.7 | 82.7 |
| C9 | Nonaylcarnitine | 86493 / 70997 / 85527 / 86054 | acylcarnitines | FIA | 14.2 | 99.9 |
| lysoPC a C14:0 | | 64483 / 64489 | glycerophospholipids | FIA | 8.1 | 99.9 |
| lysoPC a C16:0 | | 64563 / 72998 / 76078 | glycerophospholipids | FIA | 11.1 | 0 |
| lysoPC a C16:1 | | 64560 / 73851 / 84752 | glycerophospholipids | FIA | 11.1 | 0 |

| Metabolite short name | Common name | ChEBI ID | Class | Assay | CV % | % BLD |
|---|---|---|---|---|---|---|
| lysoPC a C17:0 | | 72737 / 74340 | glycerophospholipids | FIA | 10.8 | 0 |
| lysoPC a C18:0 | | 64561 / 73858 / 76076 | glycerophospholipids | FIA | 11.4 | 0 |
| lysoPC a C18:1 | | 64566 / 72589 / 76083 / 86255 | glycerophospholipids | FIA | 11 | 0 |
| lysoPC a C18:2 | | 64549 / 28733 / 76084 | glycerophospholipids | FIA | 11 | 0 |
| lysoPC a C20:3 | | 64481 / 64488 / 74343 / 86256 | glycerophospholipids | FIA | 10.8 | 0 |
| lysoPC a C20:4 | | 64568 / 74344 / 76079 / 86259 | glycerophospholipids | FIA | 10.7 | 0 |
| lysoPC a C24:0 | | 74470 / 86260 | glycerophospholipids | FIA | 35.8 | 0 |
| lysoPC a C26:0 | | 74472 | glycerophospholipids | FIA | 56 | 0 |
| lysoPC a C26:1 | | 74473 | glycerophospholipids | FIA | 58 | 0.6 |
| lysoPC a C28:0 | | 85561 | glycerophospholipids | FIA | 37.5 | 0.3 |
| lysoPC a C28:1 | | 85562 | glycerophospholipids | FIA | 43 | 0 |
| PC aa C24:0 | | 85564 / 65211 / 75302 / 86276 / 86278 / 86280 / 86281 / 86282 | glycerophospholipids | FIA | 51 | 1 |
| PC aa C26:0 (#) | | Not Available | glycerophospholipids | FIA | 42.5 | 60.1 |
| PC aa C28:1 | | 65293 / 86410 | glycerophospholipids | FIA | 10.9 | 0 |
| PC aa C30:0 | | 65303 / 75062 / 75304 / 86088 | glycerophospholipids | FIA | 8.2 | 0 |
| PC aa C30:2 | | 65301 / 86415 | glycerophospholipids | FIA | 56.4 | 14.6 |
| PC aa C32:0 | | 66850 / 72999 / 86089 / 86090 | glycerophospholipids | FIA | 12.7 | 0 |
| PC aa C32:1 | | 66849 / 73793 / 74000 / 84808 / 86092 | glycerophospholipids | FIA | 13.3 | 0 |
| PC aa C32:2 | | 66848 / 83717 | glycerophospholipids | FIA | 14.9 | 0 |
| PC aa C32:3 | | 66847 / 86095 | glycerophospholipids | FIA | 14.7 | 0 |
| PC aa C34:1 | | 64517 / 73001 / 74667 / 84570 / 85037 / 86097 | glycerophospholipids | FIA | 12.2 | 0 |
| PC aa C34:2 | | 64516 / 73002 / 84785 / 84809 / 84810 / 84811 / 86099 / 86100 | glycerophospholipids | FIA | 12.7 | 0 |
| PC aa C34:3 | | 64424 / 84567 / 84786 / 84789 | glycerophospholipids | FIA | 13.1 | 0 |
| PC aa C34:4 | | 64423 / 86101 / 86102 | glycerophospholipids | FIA | 13.7 | 0 |
| PC aa C36:0 | | 66858 / 75294 / 83718 / 86103 / 86106 / 86107 | glycerophospholipids | FIA | 13.4 | 0 |
| PC aa C36:1 | | 66857 / 76073 / 84575 / 84818 | glycerophospholipids | FIA | 11.1 | 0 |
| PC aa C36:2 | | 64433 / 74669 / 84574 / 84819 / 84820 / 84821 / 84822 / 84836 / 86112 | glycerophospholipids | FIA | 11.6 | 0 |
| PC aa C36:3 | | 64523 / 74670 / 84831 / 86117 / 86119 / 86121 | glycerophospholipids | FIA | 11.9 | 0 |
| PC aa C36:4 | | 64520 / 73003 / 77694 / 84794 / 84815 / 86123 / 86127 / 86129 / 86130 / 86133 / 86134 | glycerophospholipids | FIA | 11.8 | 0 |
| PC aa C36:5 | | 64504 / 64505 / 84816 / 86137 | glycerophospholipids | FIA | 12.2 | 0 |
| PC aa C36:6 | | 66856 / 86161 / 86162 | glycerophospholipids | FIA | 14.6 | 0 |
| PC aa C38:0 | | 66861 / 86163 / 86164 / 86166 / 86167 / 86168 / 86169 | glycerophospholipids | FIA | 10.7 | 0 |
| PC aa C38:1 | | 66860 / 86170 / 86171 / 86173 / 86174 / 86175 | glycerophospholipids | FIA | 32.2 | 0 |
| PC aa C38:3 | | 64446 / 74479 / 86176 / 86177 | glycerophospholipids | FIA | 11.1 | 0 |
| PC aa C38:4 | | 64526 / 74965 / 84573 / 84823 / 86178 | glycerophospholipids | FIA | 11.2 | 0 |
| PC aa C38:5 | | 64525 / 74671 / 84795 / 84796 / 86181 | glycerophospholipids | FIA | 11 | 0 |
| PC aa C38:6 | | 64519 / 74963 / 84563 / 84797 / 86182 / 86183 / 86184 / 86186 / 86187 | glycerophospholipids | FIA | 11.3 | 0 |
| PC aa C40:1 | | 66865 / 86188 / 86189 / 86190 / 86196 / 86197 | glycerophospholipids | FIA | 12 | 64.9 |
| PC aa C40:2 | | 66864 / 86198 / 86199 | glycerophospholipids | FIA | 13.9 | 0 |
| PC aa C40:3 | | 66863 / 86416 | glycerophospholipids | FIA | 13.8 | 0 |
| PC aa C40:4 | | 66862 / 74970 / 84565 / 86200 | glycerophospholipids | FIA | 10.2 | 0 |
| PC aa C40:5 | | 64524 / 73865 / 84151 / 86201 / 86203 | glycerophospholipids | FIA | 11 | 0 |
| PC aa C40:6 | | 64431 / 73868 / 84829 / 84830 / 86205 | glycerophospholipids | FIA | 10.4 | 0 |
| PC aa C42:0 | | 66971 / 86208 / 86210 / 86211 / 86212 | glycerophospholipids | FIA | 10.7 | 0 |

| Metabolite short name | Common name | ChEBI ID | Class | Assay | CV % | % BLD |
|---|---|---|---|---|---|---|
| PC aa C42:1 | | 66970 / 86213 / 86215 / 86216 / 86217 / 86219 | glycerophospholipids | FIA | 13.9 | 0 |
| PC aa C42:2 | | 66969 / 86418 | glycerophospholipids | FIA | 14.7 | 0 |
| PC aa C42:4 | | 66967 / 86422 | glycerophospholipids | FIA | 13.7 | 0 |
| PC aa C42:5 | | 66966 / 86220 | glycerophospholipids | FIA | 10.7 | 0 |
| PC aa C42:6 | | 66965 / 86221 | glycerophospholipids | FIA | 11 | 2.4 |
| PC ae C30:0 | | 85565 | glycerophospholipids | FIA | 15.9 | 0.1 |
| PC ae C30:1 | | 85566 / 86225 | glycerophospholipids | FIA | 53.5 | 0 |
| PC ae C30:2 | | 85567 / 86423 | glycerophospholipids | FIA | 32.9 | 0 |
| PC ae C32:1 | | 72347 / 86424 | glycerophospholipids | FIA | 14.2 | 0 |
| PC ae C32:2 | | 85568 / 86425 | glycerophospholipids | FIA | 16.3 | 0 |
| PC ae C34:0 | | 67077 / 86229 | glycerophospholipids | FIA | 12.8 | 0 |
| PC ae C34:1 | | 67076 / 84825 | glycerophospholipids | FIA | 12.9 | 0 |
| PC ae C34:2 | | 64544 / 86231 | glycerophospholipids | FIA | 13.3 | 0 |
| PC ae C34:3 | | 64541 / 86427 | glycerophospholipids | FIA | 13.2 | 0 |
| PC ae C36:0 | | 67067 / 86239 / 86240 | glycerophospholipids | FIA | 12.7 | 0 |
| PC ae C36:1 | | 67066 / 86432 | glycerophospholipids | FIA | 11.1 | 0 |
| PC ae C36:2 | | 67065 / 86504 | glycerophospholipids | FIA | 11.7 | 0 |
| PC ae C36:3 | | 64537 / 86436 | glycerophospholipids | FIA | 12.4 | 0 |
| PC ae C36:4 | | 67064 / 55430 | glycerophospholipids | FIA | 12.2 | 0 |
| PC ae C36:5 | | 64540 / 86437 | glycerophospholipids | FIA | 12.6 | 0 |
| PC ae C38:0 | | 67071 / 74482 / 86243 | glycerophospholipids | FIA | 11.5 | 0 |
| PC ae C38:1 | | 67070 / 86438 | glycerophospholipids | FIA | 29.3 | 0.5 |
| PC ae C38:2 | | 67069 / 86439 | glycerophospholipids | FIA | 11.9 | 0 |
| PC ae C38:3 | | 67068 / 86442 | glycerophospholipids | FIA | 10.7 | 0 |
| PC ae C38:4 | | 64480 / 86245 | glycerophospholipids | FIA | 12.1 | 0 |
| PC ae C38:5 | | 64445 | glycerophospholipids | FIA | 11.8 | 0 |
| PC ae C38:6 | | 64536 / 86248 | glycerophospholipids | FIA | 11.6 | 0 |
| PC ae C40:1 | | 85574 / 86443 | glycerophospholipids | FIA | 16.9 | 0 |
| PC ae C40:2 | | 72348 / 86444 | glycerophospholipids | FIA | 10.5 | 0 |
| PC ae C40:3 | | 85570 / 86445 | glycerophospholipids | FIA | 11.2 | 0 |
| PC ae C40:4 | | 85571 / 86447 | glycerophospholipids | FIA | 9.9 | 0 |
| PC ae C40:5 | | 85573 / 86448 | glycerophospholipids | FIA | 11.7 | 0 |
| PC ae C40:6 | | 64533 / 86252 | glycerophospholipids | FIA | 11.6 | 0 |
| PC ae C42:0 | | 86253 / 85582 | glycerophospholipids | FIA | 10.6 | 99.9 |
| PC ae C42:1 | | 85583 / 86449 | glycerophospholipids | FIA | 25 | 10.3 |
| PC ae C42:2 | | 85584 / 86450 | glycerophospholipids | FIA | 16 | 0 |
| PC ae C42:3 | | 85585 / 86451 | glycerophospholipids | FIA | 15 | 0 |
| PC ae C42:4 | | 85588 / 86452 | glycerophospholipids | FIA | 10.3 | 0 |
| PC ae C42:5 | | 85590 | glycerophospholipids | FIA | 9 | 0 |
| PC ae C44:3 | | 67085 / 86454 | glycerophospholipids | FIA | 28.3 | 0 |
| PC ae C44:4 | | 67084 / 86456 | glycerophospholipids | FIA | 13.7 | 0 |
| PC ae C44:5 | | 67083 | glycerophospholipids | FIA | 11.1 | 0 |
| PC ae C44:6 | | 67082 | glycerophospholipids | FIA | 10.2 | 0 |
| SM (OH) C14:1 | | 85597 / 90011 | sphingolipids | FIA | 9.1 | 0 |
| SM (OH) C16:1 | | 85626 / 90007 | sphingolipids | FIA | 10 | 0 |

| Metabolite short name | Common name | ChEBI ID | Class | Assay | CV % | % BLD |
|---|---|---|---|---|---|---|
| SM (OH) C22:1 | | 85599 / 90010 | sphingolipids | FIA | 15.4 | 0 |
| SM (OH) C22:2 | | 85600 / 90003 | sphingolipids | FIA | 15.6 | 0 |
| SM (OH) C24:1 | | 85601 / 90006 | sphingolipids | FIA | 16.2 | 0 |
| SM C16:0 | | 78646 | sphingolipids | FIA | 9.1 | 0 |
| SM C16:1 | | 85592 / 64487 | sphingolipids | FIA | 9.3 | 0 |
| SM C18:0 | | 83358 | sphingolipids | FIA | 10.9 | 0 |
| SM C18:1 | | 85593 / 84487 / 86086 | sphingolipids | FIA | 10.3 | 0 |
| SM C20:2 | | 85595 | sphingolipids | FIA | 13.9 | 0 |
| SM C22:3 (#) | | Not available | sphingolipids | FIA | 62.9 | 35 |
| SM C24:0 | | 83360 | sphingolipids | FIA | 15.3 | 0 |
| SM C24:1 | | 83172 / 74535 | sphingolipids | FIA | 16.4 | 0 |
| SM C26:0 | | 83361 | sphingolipids | FIA | 27.4 | 0 |
| SM C26:1 | | 83362 / 84476 | sphingolipids | FIA | 27.1 | 0 |
| H1 | Hexose (Sugar) | 4167 / 17234 / 17925 / 28061 / 4208 / 15903 / 28645 / 10295 / 47693 / 27667 / 37704 / 4139 / 18133 / 1416 / 17011 / 24973 / 33917 / 33921 / 33984 / 4194 / 80423 / 88378 / 88746 / 88747 | sugars | FIA | 7.2 | 0 |

NB. LC-MS/MS metabolite exclusion was based on a variable meeting two conditions 1) CV of over 30%; and 2) over 30% of the data are below LOD. 11 out of the 188 serum metabolites detected were excluded as a result.# represents metabolites which were excluded from subsequent data analyses. CV for c4-OH-Pro and DOPA are not available as peaks cannot be detected and/ or integrated reproducibly with the quality control samples. DOPA and c4-OH-Pro are counted as part of the 11 exlcuded metabolites.

**Supplementary Table 4 Summary of urinary metabolite concentrations across the 6 cohorts**

| **µmol/mmol of creatinine (median with IQR)** | **BiB** (n = 199 ) | **EDEN** (n = 157 ) | **INMA** (n = 207 ) | **KANC** (n = 201 ) | **MoBa** (n = 229 ) | **Rhea** (n = 199 ) |
|---|---|---|---|---|---|---|
| creatinine (umol/L) | 6120 ( 4760 - 7920 ) | 7180 ( 6020 - 9060 ) | 6080 ( 4630 - 7810 ) | 5610 ( 4180 - 7100 ) | 5630 ( 4370 - 6800 ) | 5420 ( 4180 - 7180 ) |
| leucine | 2.61 ( 2.1 - 3.26 ) | 2.59 ( 2.14 - 3.06 ) | 3.11 ( 2.39 - 3.86 ) | 2.86 ( 2.33 - 3.42 ) | 2.83 ( 2.32 - 3.45 ) | 3.2 ( 2.56 - 3.92 ) |
| isoleucine | 1.78 ( 1.26 - 2.64 ) | 1.49 ( 1.13 - 1.89 ) | 1.68 ( 1.35 - 2.02 ) | 1.96 ( 1.4 - 2.64 ) | 1.87 ( 1.25 - 2.51 ) | 1.69 ( 1.32 - 2.08 ) |
| valine | 3.74 ( 3.2 - 4.65 ) | 3.54 ( 2.97 - 4.16 ) | 4.13 ( 3.34 - 4.98 ) | 3.96 ( 3.42 - 4.81 ) | 3.84 ( 3.27 - 4.79 ) | 4.46 ( 3.66 - 5.47 ) |
| 3-hydroxyisobutyrate | 11.9 ( 9.73 - 15.9 ) | 12.3 ( 10 - 15.1 ) | 13.7 ( 10.7 - 18.2 ) | 12.6 ( 9.82 - 16.7 ) | 12.7 ( 9.95 - 16.3 ) | 14.3 ( 10.8 - 19.1 ) |
| 4-deoxyerythronic acid | 10.1 ( 8.33 - 12.7 ) | 10.4 ( 8.78 - 13 ) | 12 ( 9.45 - 14.8 ) | 9.87 ( 7.67 - 12.2 ) | 9.33 ( 7.47 - 11.2 ) | 11.8 ( 9.33 - 15.1 ) |
| 4-deoxythreonic acid | 16.4 ( 12.9 - 20.1 ) | 19.1 ( 15.5 - 25.2 ) | 18.5 ( 15.5 - 22.4 ) | 18.4 ( 14.5 - 23.6 ) | 17.7 ( 13.9 - 24.9 ) | 19.1 ( 14.7 - 24.4 ) |
| 2-hydroxyisobutyrate | 6.29 ( 5.14 - 7.57 ) | 6.07 ( 5.15 - 7.07 ) | 6.08 ( 5.09 - 7.17 ) | 6.94 ( 5.79 - 8.08 ) | 6.18 ( 5.22 - 7.62 ) | 6.72 ( 5.55 - 8.32 ) |
| alanine | 49.9 ( 39 - 65.4 ) | 40.7 ( 33.1 - 56.3 ) | 50.9 ( 33.8 - 64.2 ) | 47.3 ( 33.8 - 60.9 ) | 44.3 ( 34.1 - 56.7 ) | 49.8 ( 37.5 - 72.3 ) |
| lysine | 33.1 ( 25.8 - 44 ) | 27.7 ( 22.3 - 39.6 ) | 36.3 ( 26.1 - 49.9 ) | 31.6 ( 25.5 - 42.8 ) | 30.6 ( 23.6 - 41.6 ) | 36.8 ( 27.4 - 51.9 ) |
| acetate | 9.17 ( 6.4 - 11.6 ) | 6.51 ( 5.26 - 8.59 ) | 7.39 ( 5.67 - 9.73 ) | 8.19 ( 6.22 - 10.4 ) | 7.84 ( 5.91 - 10.7 ) | 8.25 ( 6.8 - 10.8 ) |
| *p*-cresol sulfate | 60.2 ( 30.8 - 89.7 ) | 41.5 ( 27.4 - 62.5 ) | 46.8 ( 29.1 - 72.5 ) | 50.9 ( 29.5 - 82.2 ) | 46.9 ( 24.7 - 68.8 ) | 44.5 ( 24.1 - 75.2 ) |
| succinate | 17.3 ( 11.3 - 27.7 ) | 12.3 ( 7.44 - 16.9 ) | 15 ( 10 - 23 ) | 20.3 ( 13.9 - 28.3 ) | 18 ( 12.3 - 25.7 ) | 19.1 ( 13 - 27.1 ) |
| glutamine | 134 ( 106 - 166 ) | 125 ( 95.1 - 158 ) | 134 ( 106 - 161 ) | 134 ( 110 - 160 ) | 131 ( 111 - 163 ) | 144 ( 113 - 176 ) |
| citrate | 575 ( 388 - 808 ) | 505 ( 349 - 671 ) | 426 ( 273 - 602 ) | 418 ( 252 - 606 ) | 451 ( 325 - 637 ) | 488 ( 327 - 683 ) |
| dimethylamine | 60.2 ( 53.2 - 70.8 ) | 48 ( 43.9 - 52 ) | 52.3 ( 47.4 - 60.2 ) | 61.1 ( 53.7 - 66.6 ) | 54.8 ( 50 - 64.3 ) | 60.2 ( 52.5 - 66.1 ) |
| trimethylamine | 4.32 ( 3.08 - 6.03 ) | 3.49 ( 2.51 - 4.54 ) | 4.39 ( 3.22 - 5.66 ) | 4.71 ( 3.28 - 6.07 ) | 3.87 ( 2.96 - 5.4 ) | 4.13 ( 3.36 - 5.88 ) |
| trimethylamine *N*-oxide | 55 ( 36.6 - 94.2 ) | 66.1 ( 45.2 - 101 ) | 59.7 ( 40.3 - 110 ) | 55.3 ( 42.5 - 80.9 ) | 71.8 ( 51.3 - 117 ) | 54.2 ( 39.6 - 88.7 ) |
| *scyllo*-inositol | 8.8 ( 6.38 - 12.5 ) | 11.9 ( 7.78 - 18.4 ) | 8.91 ( 5.9 - 13.2 ) | 10.4 ( 7.37 - 14.2 ) | 9.95 ( 7.15 - 15.3 ) | 11.9 ( 9.27 - 16.9 ) |
| taurine | 115 ( 66.2 - 176 ) | 134 ( 88.9 - 189 ) | 166 ( 121 - 234 ) | 114 ( 71.3 - 181 ) | 131 ( 76 - 191 ) | 128 ( 83.8 - 186 ) |
| glyine | 111 ( 78.7 - 158 ) | 91.3 ( 70.6 - 127 ) | 98 ( 69.8 - 131 ) | 87.1 ( 62 - 131 ) | 95.1 ( 71.6 - 125 ) | 95.4 ( 68.3 - 141 ) |
| creatine | 191 ( 91.8 - 341 ) | 136 ( 44.8 - 269 ) | 298 ( 171 - 510 ) | 201 ( 100 - 372 ) | 187 ( 89.3 - 425 ) | 207 ( 124 - 354 ) |
| hippurate | 199 ( 135 - 331 ) | 194 ( 148 - 282 ) | 152 ( 108 - 251 ) | 295 ( 204 - 480 ) | 322 ( 228 - 460 ) | 173 ( 111 - 288 ) |
| formate | 21.9 ( 16.1 - 29.8 ) | 14.3 ( 10.9 - 20.6 ) | 20.1 ( 14.6 - 26.7 ) | 20.6 ( 15.6 - 27.6 ) | 19.1 ( 13.8 - 24.6 ) | 21.7 ( 16.6 - 31.1 ) |

## Supplementary Table 5 Summary of serum metabolite concentrations across the 6 cohorts

| **µmol/L (median with IQR)** | **BiB** (n = 199 ) | **EDEN** (n = 157 ) | **KANC** (n = 201 ) | **MoBa** (n = 229 ) | **Rhea** (n = 199 ) | **INMA** (n = 207 ) |
|---|---|---|---|---|---|---|
| C0 | 33.9 ( 28.8 - 38.8 ) | 36.6 ( 32.2 - 40.8 ) | 35.3 ( 31 - 39.9 ) | 35.3 ( 31 - 40.3 ) | 34.2 ( 30.7 - 40.2 ) | 36.4 ( 32.2 - 41.1 ) |
| C10 | 0.23 ( 0.186 - 0.278 ) | 0.177 ( 0.149 - 0.237 ) | 0.258 ( 0.212 - 0.299 ) | 0.216 ( 0.177 - 0.268 ) | 0.221 ( 0.184 - 0.257 ) | 0.202 ( 0.168 - 0.242 ) |
| C10:1 | 0.11 ( 0.0835 - 0.142 ) | 0.08 ( 0.067 - 0.097 ) | 0.121 ( 0.098 - 0.148 ) | 0.096 ( 0.077 - 0.116 ) | 0.1 ( 0.083 - 0.123 ) | 0.113 ( 0.088 - 0.142 ) |
| C10:2 | 0.069 ( 0.062 - 0.078 ) | 0.068 ( 0.063 - 0.074 ) | 0.063 ( 0.058 - 0.068 ) | 0.067 ( 0.061 - 0.074 ) | 0.06 ( 0.055 - 0.0655 ) | 0.059 ( 0.056 - 0.065 ) |
| C12 | 0.107 ( 0.089 - 0.13 ) | 0.086 ( 0.077 - 0.111 ) | 0.122 ( 0.103 - 0.148 ) | 0.103 ( 0.086 - 0.129 ) | 0.109 ( 0.091 - 0.126 ) | 0.098 ( 0.083 - 0.119 ) |
| C12-DC | 0.231 ( 0.215 - 0.245 ) | 0.233 ( 0.216 - 0.245 ) | 0.236 ( 0.219 - 0.248 ) | 0.23 ( 0.218 - 0.245 ) | 0.232 ( 0.218 - 0.245 ) | 0.232 ( 0.218 - 0.248 ) |
| C12:1 | 0.111 ( 0.092 - 0.134 ) | 0.094 ( 0.081 - 0.113 ) | 0.127 ( 0.103 - 0.152 ) | 0.115 ( 0.092 - 0.141 ) | 0.12 ( 0.102 - 0.137 ) | 0.107 ( 0.093 - 0.127 ) |
| C14 | 0.057 ( 0.051 - 0.062 ) | 0.055 ( 0.048 - 0.06 ) | 0.06 ( 0.055 - 0.067 ) | 0.056 ( 0.051 - 0.063 ) | 0.057 ( 0.05 - 0.063 ) | 0.056 ( 0.05 - 0.06 ) |
| C14:1 | 0.04 ( 0.03 - 0.0585 ) | 0.03 ( 0.024 - 0.046 ) | 0.048 ( 0.037 - 0.063 ) | 0.042 ( 0.028 - 0.057 ) | 0.048 ( 0.0335 - 0.064 ) | 0.041 ( 0.029 - 0.0535 ) |
| C14:1-OH | 0.017 ( 0.015 - 0.02 ) | 0.016 ( 0.015 - 0.018 ) | 0.019 ( 0.016 - 0.021 ) | 0.017 ( 0.015 - 0.02 ) | 0.018 ( 0.016 - 0.021 ) | 0.017 ( 0.015 - 0.019 ) |
| C14:2 | 0.021 ( 0.016 - 0.03 ) | 0.016 ( 0.013 - 0.021 ) | 0.024 ( 0.019 - 0.032 ) | 0.02 ( 0.014 - 0.027 ) | 0.022 ( 0.016 - 0.027 ) | 0.022 ( 0.0175 - 0.029 ) |
| C14:2-OH | 0.02 ( 0.0175 - 0.022 ) | 0.02 ( 0.017 - 0.022 ) | 0.02 ( 0.018 - 0.023 ) | 0.02 ( 0.016 - 0.022 ) | 0.02 ( 0.017 - 0.022 ) | 0.02 ( 0.0185 - 0.023 ) |
| C16 | 0.093 ( 0.08 - 0.11 ) | 0.082 ( 0.072 - 0.095 ) | 0.093 ( 0.079 - 0.11 ) | 0.08 ( 0.066 - 0.095 ) | 0.103 ( 0.09 - 0.119 ) | 0.084 ( 0.071 - 0.0945 ) |
| C16-OH | 0.044 ( 0.039 - 0.05 ) | 0.044 ( 0.04 - 0.049 ) | 0.046 ( 0.039 - 0.05 ) | 0.044 ( 0.037 - 0.049 ) | 0.045 ( 0.04 - 0.05 ) | 0.046 ( 0.042 - 0.051 ) |
| C16:1 | 0.026 ( 0.022 - 0.03 ) | 0.024 ( 0.021 - 0.027 ) | 0.027 ( 0.024 - 0.032 ) | 0.026 ( 0.022 - 0.031 ) | 0.028 ( 0.024 - 0.033 ) | 0.025 ( 0.022 - 0.029 ) |
| C16:1-OH | 0.014 ( 0.012 - 0.016 ) | 0.013 ( 0.012 - 0.015 ) | 0.015 ( 0.013 - 0.016 ) | 0.014 ( 0.012 - 0.016 ) | 0.015 ( 0.013 - 0.017 ) | 0.013 ( 0.012 - 0.015 ) |
| C16:2 | 0.015 ( 0.013 - 0.018 ) | 0.013 ( 0.012 - 0.016 ) | 0.015 ( 0.013 - 0.017 ) | 0.015 ( 0.012 - 0.016 ) | 0.015 ( 0.013 - 0.018 ) | 0.015 ( 0.013 - 0.017 ) |
| C16:2-OH | 0.026 ( 0.024 - 0.029 ) | 0.025 ( 0.023 - 0.027 ) | 0.027 ( 0.025 - 0.029 ) | 0.026 ( 0.023 - 0.027 ) | 0.026 ( 0.024 - 0.028 ) | 0.026 ( 0.024 - 0.028 ) |
| C18 | 0.042 ( 0.036 - 0.051 ) | 0.039 ( 0.034 - 0.046 ) | 0.044 ( 0.037 - 0.05 ) | 0.04 ( 0.034 - 0.046 ) | 0.044 ( 0.038 - 0.052 ) | 0.039 ( 0.033 - 0.045 ) |
| C18:1 | 0.096 ( 0.083 - 0.12 ) | 0.078 ( 0.068 - 0.092 ) | 0.092 ( 0.076 - 0.112 ) | 0.087 ( 0.073 - 0.104 ) | 0.116 ( 0.0915 - 0.138 ) | 0.092 ( 0.0785 - 0.111 ) |
| C18:2 | 0.041 ( 0.0345 - 0.0505 ) | 0.03 ( 0.026 - 0.034 ) | 0.037 ( 0.031 - 0.043 ) | 0.031 ( 0.027 - 0.037 ) | 0.04 ( 0.033 - 0.046 ) | 0.04 ( 0.034 - 0.049 ) |
| C2 | 4.76 ( 3.66 - 6.72 ) | 4.17 ( 3.49 - 5.17 ) | 5.73 ( 4.52 - 7.72 ) | 4.97 ( 3.75 - 6.92 ) | 6.15 ( 4.45 - 9.1 ) | 4.99 ( 3.88 - 6.59 ) |
| C3 | 0.207 ( 0.16 - 0.258 ) | 0.23 ( 0.185 - 0.283 ) | 0.228 ( 0.179 - 0.277 ) | 0.207 ( 0.166 - 0.263 ) | 0.216 ( 0.17 - 0.293 ) | 0.247 ( 0.198 - 0.31 ) |
| C3-DC (C4-OH) | 0.034 ( 0.028 - 0.042 ) | 0.029 ( 0.025 - 0.035 ) | 0.032 ( 0.027 - 0.04 ) | 0.03 ( 0.025 - 0.037 ) | 0.035 ( 0.03 - 0.045 ) | 0.029 ( 0.025 - 0.036 ) |
| C3-OH | 0.023 ( 0.019 - 0.029 ) | 0.022 ( 0.018 - 0.028 ) | 0.022 ( 0.019 - 0.028 ) | 0.023 ( 0.018 - 0.028 ) | 0.023 ( 0.019 - 0.029 ) | 0.022 ( 0.019 - 0.029 ) |
| C4 | 0.103 ( 0.08 - 0.133 ) | 0.111 ( 0.088 - 0.138 ) | 0.108 ( 0.086 - 0.14 ) | 0.117 ( 0.091 - 0.149 ) | 0.102 ( 0.082 - 0.138 ) | 0.119 ( 0.0915 - 0.15 ) |
| C4:1 | 0.021 ( 0.018 - 0.023 ) | 0.021 ( 0.018 - 0.024 ) | 0.021 ( 0.018 - 0.023 ) | 0.021 ( 0.018 - 0.024 ) | 0.021 ( 0.019 - 0.024 ) | 0.021 ( 0.018 - 0.023 ) |
| C6 (C4:1-DC) | 0.058 ( 0.0485 - 0.065 ) | 0.052 ( 0.044 - 0.061 ) | 0.063 ( 0.053 - 0.073 ) | 0.055 ( 0.048 - 0.065 ) | 0.058 ( 0.0505 - 0.066 ) | 0.055 ( 0.047 - 0.062 ) |
| C5 | 0.111 ( 0.0905 - 0.136 ) | 0.124 ( 0.104 - 0.153 ) | 0.119 ( 0.098 - 0.151 ) | 0.119 ( 0.101 - 0.15 ) | 0.124 ( 0.101 - 0.154 ) | 0.133 ( 0.111 - 0.17 ) |
| C5-M-DC | 0.029 ( 0.026 - 0.032 ) | 0.028 ( 0.025 - 0.031 ) | 0.029 ( 0.026 - 0.033 ) | 0.03 ( 0.027 - 0.033 ) | 0.03 ( 0.026 - 0.034 ) | 0.028 ( 0.025 - 0.031 ) |
| C5-OH (C3-DC-M) | 0.062 ( 0.058 - 0.067 ) | 0.064 ( 0.059 - 0.069 ) | 0.063 ( 0.059 - 0.068 ) | 0.064 ( 0.059 - 0.069 ) | 0.065 ( 0.06 - 0.0695 ) | 0.065 ( 0.06 - 0.069 ) |
| C5:1 | 0.04 ( 0.036 - 0.045 ) | 0.041 ( 0.036 - 0.045 ) | 0.042 ( 0.037 - 0.046 ) | 0.043 ( 0.038 - 0.049 ) | 0.043 ( 0.039 - 0.047 ) | 0.042 ( 0.038 - 0.046 ) |
| C5:1-DC | 0.027 ( 0.024 - 0.0305 ) | 0.027 ( 0.024 - 0.032 ) | 0.027 ( 0.024 - 0.032 ) | 0.028 ( 0.024 - 0.031 ) | 0.027 ( 0.024 - 0.031 ) | 0.027 ( 0.024 - 0.032 ) |
| C5-DC (C6-OH) | 0.023 ( 0.021 - 0.026 ) | 0.022 ( 0.02 - 0.024 ) | 0.023 ( 0.021 - 0.026 ) | 0.023 ( 0.02 - 0.026 ) | 0.022 ( 0.02 - 0.025 ) | 0.022 ( 0.02 - 0.024 ) |
| C6:1 | 0.022 ( 0.019 - 0.024 ) | 0.02 ( 0.018 - 0.022 ) | 0.021 ( 0.019 - 0.024 ) | 0.021 ( 0.019 - 0.024 ) | 0.02 ( 0.018 - 0.022 ) | 0.02 ( 0.018 - 0.022 ) |
| C7-DC | 0.055 ( 0.047 - 0.062 ) | 0.048 ( 0.044 - 0.055 ) | 0.054 ( 0.049 - 0.062 ) | 0.051 ( 0.046 - 0.058 ) | 0.051 ( 0.046 - 0.0575 ) | 0.051 ( 0.046 - 0.0575 ) |
| C8 | 0.137 ( 0.118 - 0.161 ) | 0.12 ( 0.107 - 0.142 ) | 0.148 ( 0.129 - 0.167 ) | 0.135 ( 0.114 - 0.16 ) | 0.134 ( 0.118 - 0.152 ) | 0.129 ( 0.11 - 0.146 ) |
| C9 | 0.061 ( 0.054 - 0.069 ) | 0.056 ( 0.05 - 0.062 ) | 0.063 ( 0.057 - 0.073 ) | 0.066 ( 0.058 - 0.078 ) | 0.058 ( 0.053 - 0.065 ) | 0.055 ( 0.0495 - 0.061 ) |
| Ala | 350 ( 292 - 400 ) | 356 ( 305 - 404 ) | 319 ( 271 - 381 ) | 304 ( 260 - 358 ) | 322 ( 273 - 384 ) | 343 ( 300 - 392 ) |
| Arg | 102 ( 89.4 - 118 ) | 107 ( 94 - 120 ) | 100 ( 86.7 - 116 ) | 97.2 ( 88.1 - 112 ) | 113 ( 98.5 - 130 ) | 103 ( 91.2 - 120 ) |
| Asn | 46.8 ( 40.8 - 54.4 ) | 49.1 ( 42.5 - 56.4 ) | 41 ( 35.6 - 49.9 ) | 44.7 ( 39.7 - 50.5 ) | 49.9 ( 42.3 - 60.2 ) | 46.7 ( 40.4 - 54.5 ) |
| Asp | 16 ( 12.8 - 18.9 ) | 10.6 ( 8.8 - 12.7 ) | 11.4 ( 9.84 - 13.2 ) | 11.2 ( 9.54 - 13 ) | 16.8 ( 14.2 - 20 ) | 12 ( 10.2 - 14.5 ) |
| Cit | 33.3 ( 28.7 - 37.5 ) | 28.8 ( 24.8 - 32.4 ) | 30.3 ( 26.9 - 34.7 ) | 30.4 ( 26.5 - 34.6 ) | 34.5 ( 29.9 - 40.8 ) | 29.3 ( 25.6 - 33.6 ) |
| Gln | 759 ( 680 - 864 ) | 771 ( 708 - 847 ) | 701 ( 638 - 775 ) | 781 ( 735 - 858 ) | 772 ( 700 - 849 ) | 701 ( 635 - 778 ) |
| Glu | 53.1 ( 36.4 - 70.1 ) | 37.4 ( 26.2 - 49.3 ) | 61.5 ( 51.1 - 72.5 ) | 38.4 ( 29.5 - 45.1 ) | 60.5 ( 50.9 - 71.2 ) | 45.1 ( 37.3 - 57.6 ) |
| Gly | 235 ( 201 - 273 ) | 216 ( 194 - 239 ) | 219 ( 187 - 250 ) | 212 ( 190 - 244 ) | 207 ( 181 - 236 ) | 202 ( 178 - 231 ) |
| His | 86.8 ( 79 - 96.4 ) | 87.1 ( 80.2 - 96.8 ) | 84 ( 77.2 - 94.3 ) | 85.1 ( 79.4 - 92.5 ) | 90.4 ( 80.8 - 97.4 ) | 85.6 ( 76.5 - 95.4 ) |
| Ile | 66.1 ( 57.2 - 82.7 ) | 72.5 ( 60.1 - 94.8 ) | 72.5 ( 59.7 - 93.9 ) | 70.4 ( 61.2 - 83.9 ) | 93.5 ( 74.3 - 123 ) | 79.8 ( 62 - 104 ) |
| Leu | 119 ( 105 - 150 ) | 132 ( 112 - 164 ) | 127 ( 106 - 159 ) | 128 ( 112 - 149 ) | 157 ( 130 - 204 ) | 141 ( 114 - 170 ) |

| µmol/L (median with IQR) | **BiB** (n = 199 ) | **EDEN** (n = 157 ) | **KANC** (n = 201 ) | **MoBa** (n = 229 ) | **Rhea** (n = 199 ) | **INMA** (n = 207 ) |
|---|---|---|---|---|---|---|
| Lys | 161 ( 132 - 194 ) | 192 ( 169 - 229 ) | 174 ( 145 - 208 ) | 165 ( 144 - 195 ) | 175 ( 144 - 222 ) | 190 ( 162 - 228 ) |
| Met | 18.1 ( 15.2 - 22.7 ) | 20.3 ( 17.1 - 24.7 ) | 18 ( 15 - 23 ) | 17.9 ( 15.9 - 21.6 ) | 20 ( 15.8 - 26.2 ) | 19.7 ( 16 - 25.4 ) |
| Orn | 61.2 ( 52.6 - 73 ) | 53.1 ( 48.1 - 64.6 ) | 55.4 ( 44.7 - 66.6 ) | 53.5 ( 46 - 61.3 ) | 67.5 ( 54.9 - 81.3 ) | 57.8 ( 48 - 68.2 ) |
| Phe | 65.6 ( 57.1 - 77.3 ) | 64.2 ( 55.9 - 72.1 ) | 61.3 ( 54.3 - 71.1 ) | 61.6 ( 55.1 - 69.8 ) | 75.1 ( 65.8 - 84.6 ) | 67.8 ( 58.4 - 79.1 ) |
| Pro | 189 ( 144 - 231 ) | 192 ( 166 - 239 ) | 186 ( 151 - 233 ) | 184 ( 151 - 230 ) | 205 ( 172 - 250 ) | 193 ( 156 - 244 ) |
| Ser | 135 ( 123 - 153 ) | 124 ( 112 - 141 ) | 135 ( 120 - 152 ) | 130 ( 118 - 143 ) | 145 ( 130 - 168 ) | 129 ( 113 - 148 ) |
| Thr | 107 ( 90.5 - 125 ) | 127 ( 108 - 149 ) | 105 ( 88.3 - 123 ) | 107 ( 94.2 - 121 ) | 116 ( 98.1 - 144 ) | 123 ( 107 - 141 ) |
| Trp | 63.4 ( 54.8 - 77.3 ) | 67.9 ( 60.1 - 80.8 ) | 66.5 ( 58.6 - 77.2 ) | 69.4 ( 61 - 75.1 ) | 77.3 ( 65.6 - 89.1 ) | 72.1 ( 61.5 - 80.2 ) |
| Tyr | 70.6 ( 59.2 - 89.9 ) | 72.8 ( 62.8 - 88.8 ) | 69.4 ( 59.5 - 88.7 ) | 69.5 ( 57.6 - 81.1 ) | 84.6 ( 68.4 - 102 ) | 78.2 ( 63.8 - 90.6 ) |
| Val | 208 ( 178 - 250 ) | 230 ( 203 - 270 ) | 223 ( 191 - 267 ) | 222 ( 198 - 256 ) | 272 ( 222 - 318 ) | 247 ( 206 - 287 ) |
| Ac-Orn | 0.569 ( 0.389 - 0.81 ) | 0.571 ( 0.372 - 0.765 ) | 0.476 ( 0.349 - 0.696 ) | 0.482 ( 0.313 - 0.642 ) | 1.2 ( 0.611 - 2.02 ) | 0.642 ( 0.39 - 1.26 ) |
| ADMA | 0.581 ( 0.528 - 0.636 ) | 0.55 ( 0.501 - 0.613 ) | 0.595 ( 0.529 - 0.656 ) | 0.531 ( 0.495 - 0.585 ) | 0.597 ( 0.544 - 0.666 ) | 0.542 ( 0.49 - 0.607 ) |
| alpha-AAA | 0.73 ( 0.554 - 0.97 ) | 0.867 ( 0.669 - 1.16 ) | 0.847 ( 0.663 - 1.08 ) | 0.809 ( 0.631 - 0.989 ) | 0.988 ( 0.708 - 1.37 ) | 1.01 ( 0.752 - 1.31 ) |
| Creatinine | 37.4 ( 33.4 - 42.8 ) | 47.5 ( 42.6 - 52.4 ) | 38.2 ( 34.5 - 42.2 ) | 42 ( 37.8 - 45.6 ) | 39.6 ( 35.7 - 46.8 ) | 42.8 ( 37.4 - 47.6 ) |
| Kynurenine | 2.4 ( 2.06 - 2.9 ) | 2.4 ( 2.12 - 2.98 ) | 2.59 ( 2.31 - 2.97 ) | 2.5 ( 2.16 - 2.93 ) | 2.53 ( 2.2 - 2.98 ) | 2.47 ( 2.17 - 2.84 ) |
| Met-SO | 1.03 ( 0.732 - 1.38 ) | 0.734 ( 0.61 - 0.91 ) | 1.23 ( 0.97 - 1.48 ) | 0.778 ( 0.673 - 0.967 ) | 1.28 ( 0.97 - 1.61 ) | 0.945 ( 0.772 - 1.22 ) |
| Putrescine | 0.106 ( 0.078 - 0.134 ) | 0.092 ( 0.074 - 0.123 ) | 0.096 ( 0.074 - 0.12 ) | 0.099 ( 0.076 - 0.13 ) | 0.111 ( 0.0875 - 0.139 ) | 0.096 ( 0.071 - 0.12 ) |
| SDMA | 0.395 ( 0.289 - 0.498 ) | 0.384 ( 0.279 - 0.477 ) | 0.426 ( 0.332 - 0.511 ) | 0.4 ( 0.306 - 0.508 ) | 0.399 ( 0.302 - 0.488 ) | 0.323 ( 0.25 - 0.44 ) |
| Serotonin | 1.34 ( 0.948 - 1.73 ) | 0.775 ( 0.488 - 1.13 ) | 0.697 ( 0.502 - 0.975 ) | 0.995 ( 0.628 - 1.41 ) | 1.16 ( 0.852 - 1.56 ) | 0.923 ( 0.604 - 1.23 ) |
| Spermidine | 0.163 ( 0.146 - 0.194 ) | 0.164 ( 0.145 - 0.176 ) | 0.155 ( 0.138 - 0.177 ) | 0.163 ( 0.142 - 0.184 ) | 0.174 ( 0.153 - 0.2 ) | 0.152 ( 0.136 - 0.168 ) |
| Spermine | 0.214 ( 0.2 - 0.228 ) | 0.208 ( 0.197 - 0.222 ) | 0.213 ( 0.203 - 0.228 ) | 0.21 ( 0.192 - 0.224 ) | 0.223 ( 0.207 - 0.236 ) | 0.208 ( 0.18 - 0.218 ) |
| t4-OH-Pro | 14.9 ( 12.9 - 18.4 ) | 17.3 ( 13.6 - 20.6 ) | 17.1 ( 14 - 21.9 ) | 15.6 ( 13.1 - 19.2 ) | 15.9 ( 13.1 - 20.7 ) | 17.6 ( 14.2 - 22.6 ) |
| Taurine | 89 ( 64.2 - 114 ) | 54.2 ( 47.3 - 66.9 ) | 53.2 ( 46.9 - 59.6 ) | 61.6 ( 50.9 - 72.6 ) | 90.7 ( 67.1 - 114 ) | 58 ( 50.6 - 76.2 ) |
| total DMA | 0.831 ( 0.763 - 0.929 ) | 0.798 ( 0.72 - 0.878 ) | 0.875 ( 0.796 - 0.932 ) | 0.804 ( 0.739 - 0.894 ) | 0.822 ( 0.764 - 0.911 ) | 0.749 ( 0.678 - 0.832 ) |
| lysoPC a C14:0 | 2.94 ( 2.68 - 3.24 ) | 3.09 ( 2.78 - 3.42 ) | 2.94 ( 2.68 - 3.3 ) | 3.03 ( 2.75 - 3.35 ) | 2.93 ( 2.67 - 3.24 ) | 2.75 ( 2.58 - 3.06 ) |
| lysoPC a C16:0 | 65.9 ( 58.6 - 81.4 ) | 61.6 ( 54.2 - 71.9 ) | 60.9 ( 52.3 - 70.3 ) | 61.3 ( 52.6 - 69.5 ) | 68.6 ( 59.8 - 77.8 ) | 60.9 ( 54 - 70.8 ) |
| lysoPC a C16:1 | 1.71 ( 1.38 - 2.13 ) | 1.8 ( 1.54 - 2.18 ) | 1.62 ( 1.4 - 1.98 ) | 1.78 ( 1.48 - 2.11 ) | 1.69 ( 1.39 - 2.1 ) | 1.59 ( 1.31 - 1.8 ) |
| lysoPC a C17:0 | 1.15 ( 0.965 - 1.41 ) | 1.22 ( 1.04 - 1.41 ) | 1.11 ( 0.904 - 1.37 ) | 1.27 ( 1.1 - 1.46 ) | 1.04 ( 0.878 - 1.26 ) | 0.999 ( 0.823 - 1.16 ) |
| lysoPC a C18:0 | 21.3 ( 18.4 - 25.7 ) | 19.8 ( 16.9 - 22.8 ) | 20 ( 16.4 - 22.6 ) | 19.8 ( 17.4 - 22.4 ) | 21 ( 18.2 - 24.2 ) | 20.6 ( 17.5 - 24 ) |
| lysoPC a C18:1 | 18.7 ( 14.9 - 23.5 ) | 16.6 ( 13.7 - 20.1 ) | 15.6 ( 13.1 - 19 ) | 17.1 ( 14.2 - 19.9 ) | 21.9 ( 18.2 - 26.4 ) | 17 ( 13.8 - 20.6 ) |
| lysoPC a C18:2 | 39.8 ( 27.8 - 51.1 ) | 33.8 ( 25.3 - 41.9 ) | 33.3 ( 26.5 - 41.6 ) | 32.3 ( 25.6 - 38.4 ) | 44.5 ( 35.7 - 55.8 ) | 38.7 ( 27.6 - 49.8 ) |
| lysoPC a C20:3 | 2.18 ( 1.62 - 2.76 ) | 1.97 ( 1.55 - 2.6 ) | 1.74 ( 1.4 - 2.18 ) | 1.81 ( 1.44 - 2.25 ) | 2.76 ( 2.29 - 3.24 ) | 2.24 ( 1.72 - 2.64 ) |
| lysoPC a C20:4 | 5.42 ( 4.16 - 6.66 ) | 5.05 ( 4.29 - 6.1 ) | 4.91 ( 4.08 - 5.65 ) | 4.54 ( 3.97 - 5.6 ) | 6.48 ( 5.26 - 7.62 ) | 5.89 ( 4.55 - 7.14 ) |
| lysoPC a C24:0 | 0.185 ( 0.152 - 0.226 ) | 0.18 ( 0.146 - 0.226 ) | 0.177 ( 0.149 - 0.217 ) | 0.194 ( 0.159 - 0.256 ) | 0.17 ( 0.141 - 0.208 ) | 0.172 ( 0.139 - 0.22 ) |
| lysoPC a C26:0 | 0.335 ( 0.26 - 0.466 ) | 0.328 ( 0.235 - 0.464 ) | 0.303 ( 0.242 - 0.443 ) | 0.307 ( 0.245 - 0.46 ) | 0.34 ( 0.266 - 0.479 ) | 0.314 ( 0.236 - 0.422 ) |
| lysoPC a C26:1 | 0.176 ( 0.128 - 0.234 ) | 0.167 ( 0.122 - 0.23 ) | 0.163 ( 0.127 - 0.23 ) | 0.185 ( 0.133 - 0.245 ) | 0.165 ( 0.126 - 0.234 ) | 0.166 ( 0.121 - 0.226 ) |
| lysoPC a C28:0 | 0.36 ( 0.3 - 0.466 ) | 0.35 ( 0.291 - 0.451 ) | 0.34 ( 0.287 - 0.438 ) | 0.357 ( 0.295 - 0.462 ) | 0.362 ( 0.316 - 0.476 ) | 0.351 ( 0.289 - 0.43 ) |
| lysoPC a C28:1 | 0.357 ( 0.29 - 0.442 ) | 0.373 ( 0.315 - 0.475 ) | 0.366 ( 0.296 - 0.456 ) | 0.384 ( 0.32 - 0.473 ) | 0.35 ( 0.284 - 0.446 ) | 0.35 ( 0.279 - 0.408 ) |
| PC aa C24:0 | 0.148 ( 0.116 - 0.218 ) | 0.146 ( 0.115 - 0.201 ) | 0.146 ( 0.113 - 0.195 ) | 0.148 ( 0.117 - 0.206 ) | 0.152 ( 0.112 - 0.198 ) | 0.154 ( 0.118 - 0.198 ) |
| PC aa C28:1 | 2.11 ( 1.74 - 2.52 ) | 2.4 ( 2.07 - 2.81 ) | 2.13 ( 1.87 - 2.62 ) | 2.53 ( 2.21 - 2.83 ) | 2.13 ( 1.84 - 2.54 ) | 2.05 ( 1.74 - 2.46 ) |
| PC aa C30:0 | 3.32 ( 2.71 - 3.88 ) | 3.67 ( 3.18 - 4.43 ) | 3.41 ( 2.86 - 4.21 ) | 3.59 ( 3.04 - 4.45 ) | 3.41 ( 2.9 - 4.24 ) | 2.94 ( 2.37 - 3.52 ) |
| PC aa C30:2 | 0.13 ( 0.053 - 0.202 ) | 0.114 ( 0.049 - 0.187 ) | 0.113 ( 0.036 - 0.199 ) | 0.141 ( 0.06 - 0.195 ) | 0.117 ( 0.053 - 0.206 ) | 0.128 ( 0.044 - 0.21 ) |
| PC aa C32:0 | 20.9 ( 18.4 - 24.5 ) | 21.3 ( 19.1 - 23.9 ) | 21.4 ( 19.1 - 24.5 ) | 21.5 ( 18.9 - 24 ) | 23.5 ( 21.2 - 26.8 ) | 20.6 ( 17.8 - 23.2 ) |
| PC aa C32:1 | 19.9 ( 14.9 - 25 ) | 22.1 ( 18.3 - 27.9 ) | 20.1 ( 16.5 - 25.6 ) | 22 ( 17.3 - 28.4 ) | 19.4 ( 15.2 - 25.2 ) | 16.7 ( 12.4 - 21.2 ) |
| PC aa C32:2 | 6.4 ( 5.07 - 7.96 ) | 6.87 ( 5.41 - 9.04 ) | 6.42 ( 4.99 - 8.02 ) | 6.62 ( 5.05 - 8.13 ) | 6.11 ( 4.65 - 7.4 ) | 6.06 ( 4.72 - 7.92 ) |
| PC aa C32:3 | 0.788 ( 0.68 - 0.966 ) | 0.842 ( 0.711 - 1.03 ) | 0.801 ( 0.702 - 0.918 ) | 0.888 ( 0.771 - 1.08 ) | 0.734 ( 0.632 - 0.84 ) | 0.732 ( 0.638 - 0.86 ) |
| PC aa C34:1 | 323 ( 274 - 396 ) | 325 ( 277 - 373 ) | 304 ( 267 - 344 ) | 326 ( 276 - 379 ) | 369 ( 306 - 418 ) | 289 ( 251 - 342 ) |
| PC aa C34:2 | 807 ( 699 - 948 ) | 759 ( 656 - 856 ) | 788 ( 685 - 882 ) | 707 ( 624 - 806 ) | 870 ( 754 - 994 ) | 799 ( 704 - 914 ) |
| PC aa C34:3 | 26.8 ( 22.2 - 32.4 ) | 24.1 ( 19.8 - 29.7 ) | 23.5 ( 19.5 - 27.7 ) | 25.2 ( 21.7 - 30.1 ) | 21.3 ( 18 - 25 ) | 19 ( 16.8 - 23.3 ) |
| PC aa C34:4 | 2.52 ( 1.96 - 3 ) | 2.81 ( 2.27 - 3.61 ) | 2.39 ( 1.91 - 2.95 ) | 2.66 ( 2.15 - 3.29 ) | 2.41 ( 1.94 - 3 ) | 2.53 ( 1.99 - 3.06 ) |
| PC aa C36:0 | 3.6 ( 3.08 - 4.34 ) | 4.08 ( 3.56 - 4.86 ) | 3.87 ( 3.21 - 4.63 ) | 4.58 ( 3.94 - 5.51 ) | 3.58 ( 2.9 - 4.27 ) | 3.89 ( 3.33 - 4.54 ) |

| µmol/L (median with IQR) | **BiB** (n = 199 ) | **EDEN** (n = 157 ) | **KANC** (n = 201 ) | **MoBa** (n = 229 ) | **Rhea** (n = 199 ) | **INMA** (n = 207 ) |
|---|---|---|---|---|---|---|
| PC aa C36:1 | 59.2 ( 49.7 - 72.2 ) | 61.5 ( 52.3 - 72.3 ) | 56.1 ( 46.8 - 66.8 ) | 65.4 ( 54.3 - 76.2 ) | 66.6 ( 55.6 - 78.2 ) | 57.7 ( 48.8 - 67.3 ) |
| PC aa C36:2 | 423 ( 364 - 502 ) | 408 ( 350 - 455 ) | 419 ( 363 - 468 ) | 398 ( 354 - 453 ) | 440 ( 390 - 494 ) | 442 ( 392 - 506 ) |
| PC aa C36:3 | 198 ( 174 - 233 ) | 194 ( 164 - 219 ) | 186 ( 159 - 212 ) | 185 ( 165 - 215 ) | 220 ( 194 - 252 ) | 204 ( 178 - 234 ) |
| PC aa C36:4 | 255 ( 212 - 296 ) | 257 ( 229 - 294 ) | 246 ( 218 - 275 ) | 231 ( 205 - 267 ) | 283 ( 241 - 332 ) | 277 ( 234 - 326 ) |
| PC aa C36:5 | 25.5 ( 19.5 - 33.8 ) | 25.2 ( 20.3 - 32.4 ) | 20.6 ( 16.2 - 26.7 ) | 36.2 ( 28.5 - 54.2 ) | 16.1 ( 12.6 - 20.7 ) | 14.6 ( 11.1 - 19.8 ) |
| PC aa C36:6 | 1.11 ( 0.882 - 1.48 ) | 1.42 ( 1.14 - 1.75 ) | 1.07 ( 0.851 - 1.42 ) | 1.77 ( 1.41 - 2.27 ) | 0.897 ( 0.734 - 1.1 ) | 1 ( 0.799 - 1.2 ) |
| PC aa C38:0 | 3.21 ( 2.59 - 3.91 ) | 3.81 ( 3.14 - 4.45 ) | 3.63 ( 3.12 - 4.44 ) | 4.69 ( 3.99 - 5.43 ) | 3.19 ( 2.66 - 3.8 ) | 3.98 ( 3.2 - 4.58 ) |
| PC aa C38:1 | 1.21 ( 1.01 - 1.54 ) | 1.24 ( 0.991 - 1.54 ) | 1.2 ( 0.978 - 1.48 ) | 1.67 ( 1.38 - 2.03 ) | 1.16 ( 0.888 - 1.43 ) | 1.14 ( 0.878 - 1.44 ) |
| PC aa C38:3 | 56.6 ( 46 - 66.7 ) | 58.1 ( 49.2 - 69.9 ) | 50.8 ( 42.9 - 58.8 ) | 55.4 ( 48 - 65.3 ) | 59.7 ( 52.1 - 71 ) | 59.9 ( 51.3 - 70.4 ) |
| PC aa C38:4 | 129 ( 104 - 150 ) | 133 ( 118 - 150 ) | 126 ( 109 - 148 ) | 124 ( 105 - 140 ) | 137 ( 116 - 162 ) | 149 ( 124 - 176 ) |
| PC aa C38:5 | 61.2 ( 50.7 - 73.6 ) | 59.2 ( 52.4 - 67.4 ) | 57 ( 48.9 - 67 ) | 67.7 ( 58.1 - 78.3 ) | 55.4 ( 47.4 - 63.8 ) | 51.5 ( 43.2 - 62.8 ) |
| PC aa C38:6 | 80.8 ( 66.4 - 98.6 ) | 95.2 ( 79.5 - 111 ) | 80.5 ( 67.1 - 98.2 ) | 118 ( 98.5 - 142 ) | 69.8 ( 58.6 - 86.6 ) | 80.7 ( 67.4 - 95.4 ) |
| PC aa C40:1 | 0.494 ( 0.441 - 0.568 ) | 0.472 ( 0.428 - 0.532 ) | 0.497 ( 0.455 - 0.551 ) | 0.564 ( 0.503 - 0.628 ) | 0.466 ( 0.414 - 0.51 ) | 0.499 ( 0.444 - 0.562 ) |
| PC aa C40:2 | 0.391 ( 0.332 - 0.46 ) | 0.354 ( 0.309 - 0.4 ) | 0.361 ( 0.33 - 0.407 ) | 0.404 ( 0.353 - 0.473 ) | 0.356 ( 0.322 - 0.406 ) | 0.367 ( 0.317 - 0.431 ) |
| PC aa C40:3 | 0.593 ( 0.496 - 0.677 ) | 0.544 ( 0.488 - 0.61 ) | 0.54 ( 0.471 - 0.6 ) | 0.613 ( 0.557 - 0.696 ) | 0.546 ( 0.49 - 0.625 ) | 0.537 ( 0.469 - 0.61 ) |
| PC aa C40:4 | 3.73 ( 3.12 - 4.42 ) | 3.69 ( 3.19 - 4.37 ) | 3.8 ( 3.3 - 4.35 ) | 3.54 ( 3.1 - 4.1 ) | 4.05 ( 3.46 - 4.68 ) | 4.12 ( 3.42 - 4.88 ) |
| PC aa C40:5 | 9.82 ( 7.92 - 11.7 ) | 9.52 ( 8.08 - 11.2 ) | 9.31 ( 8.11 - 10.7 ) | 9.48 ( 8.09 - 11.3 ) | 8.45 ( 7.38 - 9.86 ) | 7.98 ( 6.58 - 9.59 ) |
| PC aa C40:6 | 24.7 ( 20.4 - 30.2 ) | 30 ( 24.2 - 34.6 ) | 24.6 ( 20.2 - 29.8 ) | 36.2 ( 30.5 - 44.3 ) | 20.3 ( 17.2 - 25 ) | 25.2 ( 20.6 - 29.4 ) |
| PC aa C42:0 | 0.539 ( 0.444 - 0.65 ) | 0.551 ( 0.485 - 0.634 ) | 0.557 ( 0.484 - 0.64 ) | 0.647 ( 0.555 - 0.764 ) | 0.506 ( 0.432 - 0.604 ) | 0.552 ( 0.474 - 0.653 ) |
| PC aa C42:1 | 0.286 ( 0.244 - 0.34 ) | 0.288 ( 0.24 - 0.333 ) | 0.29 ( 0.248 - 0.336 ) | 0.328 ( 0.276 - 0.388 ) | 0.261 ( 0.226 - 0.308 ) | 0.308 ( 0.255 - 0.36 ) |
| PC aa C42:2 | 0.24 ( 0.204 - 0.277 ) | 0.226 ( 0.201 - 0.252 ) | 0.215 ( 0.188 - 0.25 ) | 0.252 ( 0.229 - 0.293 ) | 0.203 ( 0.183 - 0.24 ) | 0.233 ( 0.196 - 0.264 ) |
| PC aa C42:4 | 0.171 ( 0.152 - 0.202 ) | 0.172 ( 0.15 - 0.193 ) | 0.174 ( 0.156 - 0.196 ) | 0.171 ( 0.151 - 0.193 ) | 0.177 ( 0.154 - 0.199 ) | 0.181 ( 0.156 - 0.208 ) |
| PC aa C42:5 | 0.35 ( 0.292 - 0.428 ) | 0.322 ( 0.281 - 0.372 ) | 0.341 ( 0.305 - 0.384 ) | 0.371 ( 0.326 - 0.431 ) | 0.277 ( 0.236 - 0.31 ) | 0.261 ( 0.226 - 0.3 ) |
| PC aa C42:6 | 0.554 ( 0.489 - 0.643 ) | 0.517 ( 0.457 - 0.601 ) | 0.52 ( 0.453 - 0.614 ) | 0.675 ( 0.602 - 0.782 ) | 0.45 ( 0.394 - 0.514 ) | 0.451 ( 0.398 - 0.515 ) |
| PC ae C30:0 | 0.347 ( 0.294 - 0.422 ) | 0.436 ( 0.373 - 0.505 ) | 0.416 ( 0.357 - 0.495 ) | 0.423 ( 0.348 - 0.492 ) | 0.371 ( 0.318 - 0.443 ) | 0.327 ( 0.278 - 0.396 ) |
| PC ae C30:1 | 0.24 ( 0.179 - 0.366 ) | 0.289 ( 0.204 - 0.369 ) | 0.268 ( 0.178 - 0.357 ) | 0.291 ( 0.212 - 0.38 ) | 0.258 ( 0.201 - 0.35 ) | 0.254 ( 0.19 - 0.344 ) |
| PC ae C30:2 | 0.088 ( 0.072 - 0.112 ) | 0.098 ( 0.084 - 0.12 ) | 0.092 ( 0.078 - 0.11 ) | 0.099 ( 0.084 - 0.115 ) | 0.084 ( 0.07 - 0.105 ) | 0.088 ( 0.075 - 0.105 ) |
| PC ae C32:1 | 4.55 ( 3.74 - 5.34 ) | 4.99 ( 4.4 - 5.63 ) | 4.82 ( 4.35 - 5.63 ) | 4.72 ( 4.02 - 5.58 ) | 5.3 ( 4.28 - 5.92 ) | 4.73 ( 4.11 - 5.38 ) |
| PC ae C32:2 | 1.04 ( 0.851 - 1.24 ) | 1.2 ( 1.04 - 1.35 ) | 1.1 ( 0.983 - 1.29 ) | 1.23 ( 1.08 - 1.42 ) | 1.09 ( 0.944 - 1.31 ) | 1.12 ( 0.968 - 1.29 ) |
| PC ae C34:0 | 1.93 ( 1.6 - 2.36 ) | 2.35 ( 1.96 - 2.79 ) | 2.12 ( 1.78 - 2.52 ) | 2.36 ( 2.01 - 2.76 ) | 2.02 ( 1.73 - 2.4 ) | 1.83 ( 1.49 - 2.16 ) |
| PC ae C34:1 | 16 ( 13.1 - 18.6 ) | 16.9 ( 15 - 19.4 ) | 16.6 ( 14.7 - 19.1 ) | 17.1 ( 15.1 - 19.1 ) | 17.8 ( 15.3 - 19.8 ) | 15.5 ( 13 - 17.4 ) |
| PC ae C34:2 | 19 ( 15.9 - 22.6 ) | 20.3 ( 17.6 - 23.7 ) | 21.8 ( 18.4 - 26 ) | 19.4 ( 16.7 - 22.5 ) | 21.7 ( 18.3 - 25.6 ) | 22.5 ( 19 - 26.6 ) |
| PC ae C34:3 | 15.7 ( 13.2 - 19.2 ) | 16.3 ( 13.9 - 18.8 ) | 16.6 ( 14.3 - 19.6 ) | 15.3 ( 12.9 - 18 ) | 17.6 ( 14.4 - 20.6 ) | 17.3 ( 13.8 - 20.4 ) |
| PC ae C36:0 | 1.18 ( 0.989 - 1.38 ) | 1.27 ( 1.12 - 1.4 ) | 1.16 ( 1.03 - 1.34 ) | 1.36 ( 1.19 - 1.57 ) | 1.24 ( 1.08 - 1.4 ) | 1.16 ( 1 - 1.33 ) |
| PC ae C36:1 | 10.3 ( 8.49 - 12.6 ) | 11.2 ( 9.94 - 13 ) | 10.6 ( 8.89 - 12.1 ) | 11.8 ( 10.2 - 13.4 ) | 10.4 ( 8.72 - 12.2 ) | 9.25 ( 8.06 - 10.7 ) |
| PC ae C36:2 | 21 ( 17.6 - 25.3 ) | 21.8 ( 19.6 - 25.6 ) | 22.8 ( 19.4 - 25.6 ) | 23 ( 20.1 - 25.9 ) | 20.7 ( 18 - 24.2 ) | 20.4 ( 17.8 - 23.4 ) |
| PC ae C36:3 | 12.5 ( 10.6 - 15.2 ) | 13.2 ( 11.7 - 14.9 ) | 13.7 ( 11.8 - 16 ) | 13.3 ( 11.7 - 15.2 ) | 14.4 ( 12.2 - 17.3 ) | 14.8 ( 12.6 - 17.3 ) |
| PC ae C36:4 | 24.1 ( 20.8 - 28.2 ) | 29.2 ( 25.7 - 33.2 ) | 30 ( 25.7 - 36.2 ) | 24.9 ( 21.6 - 29.8 ) | 31.7 ( 25.8 - 37 ) | 33.7 ( 28.4 - 40.2 ) |
| PC ae C36:5 | 16.2 ( 13.2 - 18.8 ) | 19.5 ( 15.9 - 23.1 ) | 18.1 ( 15.2 - 21.9 ) | 17.2 ( 14.8 - 20.8 ) | 19 ( 15.6 - 22.4 ) | 20.5 ( 16.5 - 23.7 ) |
| PC ae C38:0 | 2.29 ( 1.94 - 2.83 ) | 2.66 ( 2.22 - 2.9 ) | 2.22 ( 1.84 - 2.62 ) | 3.27 ( 2.74 - 4.04 ) | 1.84 ( 1.62 - 2.2 ) | 2.03 ( 1.69 - 2.31 ) |
| PC ae C38:1 | 0.728 ( 0.566 - 0.995 ) | 0.694 ( 0.563 - 0.876 ) | 0.655 ( 0.513 - 0.821 ) | 0.862 ( 0.677 - 1.05 ) | 0.631 ( 0.463 - 0.838 ) | 0.663 ( 0.484 - 0.876 ) |
| PC ae C38:2 | 2.91 ( 2.48 - 3.56 ) | 2.81 ( 2.38 - 3.17 ) | 2.94 ( 2.46 - 3.43 ) | 3.08 ( 2.66 - 3.43 ) | 2.98 ( 2.56 - 3.34 ) | 2.79 ( 2.44 - 3.22 ) |
| PC ae C38:3 | 5.39 ( 4.38 - 6.36 ) | 5.59 ( 4.98 - 6.53 ) | 5.15 ( 4.53 - 6.05 ) | 5.72 ( 4.97 - 6.44 ) | 5.56 ( 4.66 - 6.33 ) | 5.26 ( 4.54 - 5.92 ) |
| PC ae C38:4 | 17.8 ( 15.2 - 20.8 ) | 20.1 ( 18 - 22.4 ) | 20.6 ( 17.9 - 23.5 ) | 18.8 ( 16.1 - 21.6 ) | 20.7 ( 17.5 - 24.1 ) | 20.9 ( 17.6 - 24 ) |
| PC ae C38:5 | 22.9 ( 19.8 - 27 ) | 25.5 ( 22.9 - 28.9 ) | 26.9 ( 23.2 - 30.9 ) | 25.7 ( 22.1 - 29.6 ) | 28 ( 23.6 - 32.9 ) | 29.4 ( 24.7 - 35.2 ) |
| PC ae C38:6 | 8.35 ( 7 - 10.2 ) | 10.5 ( 8.91 - 12.1 ) | 9.7 ( 8.38 - 12.2 ) | 11.4 ( 9.51 - 13.4 ) | 8.94 ( 7.28 - 10.7 ) | 10.5 ( 8.43 - 12.4 ) |
| PC ae C40:1 | 1.41 ( 1.19 - 1.76 ) | 1.5 ( 1.31 - 1.73 ) | 1.35 ( 1.09 - 1.55 ) | 1.7 ( 1.45 - 1.93 ) | 1.37 ( 1.17 - 1.67 ) | 1.46 ( 1.26 - 1.73 ) |
| PC ae C40:2 | 1.62 ( 1.36 - 1.94 ) | 1.66 ( 1.46 - 1.86 ) | 1.59 ( 1.39 - 1.86 ) | 1.94 ( 1.68 - 2.28 ) | 1.43 ( 1.24 - 1.62 ) | 1.3 ( 1.12 - 1.46 ) |
| PC ae C40:3 | 1.23 ( 1.02 - 1.43 ) | 1.15 ( 1.04 - 1.3 ) | 1.17 ( 1.03 - 1.29 ) | 1.24 ( 1.13 - 1.41 ) | 1.19 ( 1.07 - 1.34 ) | 1.16 ( 1 - 1.32 ) |
| PC ae C40:4 | 2.7 ( 2.31 - 3.2 ) | 2.87 ( 2.46 - 3.13 ) | 2.92 ( 2.62 - 3.34 ) | 2.68 ( 2.35 - 3.06 ) | 3 ( 2.56 - 3.45 ) | 2.89 ( 2.51 - 3.34 ) |
| PC ae C40:5 | 4.32 ( 3.62 - 4.98 ) | 4.36 ( 3.81 - 4.93 ) | 4.57 ( 4.09 - 5.23 ) | 4.58 ( 4.09 - 5.26 ) | 4.46 ( 3.84 - 5.02 ) | 4.5 ( 3.74 - 5.13 ) |

| µmol/L (median with IQR) | **BiB** (n = 199 ) | **EDEN** (n = 157 ) | **KANC** (n = 201 ) | **MoBa** (n = 229 ) | **Rhea** (n = 199 ) | **INMA** (n = 207 ) |
|---|---|---|---|---|---|---|
| PC ae C40:6 | 5.13 ( 4.07 - 5.75 ) | 5.89 ( 5.03 - 6.79 ) | 5.57 ( 4.93 - 6.64 ) | 7.01 ( 6.05 - 8.27 ) | 4.71 ( 4.06 - 5.58 ) | 5.24 ( 4.53 - 6.06 ) |
| PC ae C42:0 | 0.837 ( 0.79 - 0.928 ) | 0.817 ( 0.759 - 0.874 ) | 0.822 ( 0.763 - 0.886 ) | 0.913 ( 0.854 - 0.984 ) | 0.789 ( 0.745 - 0.858 ) | 0.816 ( 0.758 - 0.88 ) |
| PC ae C42:1 | 0.493 ( 0.424 - 0.594 ) | 0.465 ( 0.407 - 0.535 ) | 0.466 ( 0.405 - 0.541 ) | 0.5 ( 0.433 - 0.565 ) | 0.474 ( 0.417 - 0.559 ) | 0.525 ( 0.444 - 0.605 ) |
| PC ae C42:2 | 0.591 ( 0.494 - 0.719 ) | 0.579 ( 0.499 - 0.65 ) | 0.569 ( 0.485 - 0.658 ) | 0.676 ( 0.565 - 0.771 ) | 0.556 ( 0.487 - 0.636 ) | 0.511 ( 0.436 - 0.588 ) |
| PC ae C42:3 | 0.83 ( 0.704 - 0.981 ) | 0.772 ( 0.683 - 0.884 ) | 0.76 ( 0.664 - 0.87 ) | 0.919 ( 0.799 - 1.06 ) | 0.765 ( 0.639 - 0.884 ) | 0.77 ( 0.658 - 0.88 ) |
| PC ae C42:4 | 0.857 ( 0.734 - 1.03 ) | 0.859 ( 0.742 - 0.986 ) | 0.911 ( 0.81 - 1.04 ) | 0.852 ( 0.753 - 0.986 ) | 0.906 ( 0.746 - 1.04 ) | 0.871 ( 0.736 - 1.01 ) |
| PC ae C42:5 | 1.98 ( 1.65 - 2.36 ) | 2.03 ( 1.82 - 2.3 ) | 2.09 ( 1.82 - 2.42 ) | 2.14 ( 1.87 - 2.48 ) | 2.07 ( 1.78 - 2.37 ) | 2.13 ( 1.75 - 2.44 ) |
| PC ae C44:3 | 0.158 ( 0.13 - 0.184 ) | 0.149 ( 0.129 - 0.179 ) | 0.149 ( 0.125 - 0.168 ) | 0.163 ( 0.137 - 0.186 ) | 0.144 ( 0.119 - 0.17 ) | 0.148 ( 0.126 - 0.179 ) |
| PC ae C44:4 | 0.324 ( 0.284 - 0.39 ) | 0.33 ( 0.298 - 0.379 ) | 0.333 ( 0.288 - 0.381 ) | 0.347 ( 0.299 - 0.393 ) | 0.347 ( 0.3 - 0.4 ) | 0.319 ( 0.278 - 0.373 ) |
| PC ae C44:5 | 1.33 ( 1.09 - 1.6 ) | 1.43 ( 1.21 - 1.69 ) | 1.41 ( 1.2 - 1.63 ) | 1.43 ( 1.23 - 1.73 ) | 1.44 ( 1.22 - 1.68 ) | 1.44 ( 1.16 - 1.68 ) |
| PC ae C44:6 | 0.968 ( 0.815 - 1.17 ) | 0.979 ( 0.821 - 1.17 ) | 1.07 ( 0.894 - 1.24 ) | 1.07 ( 0.902 - 1.26 ) | 0.945 ( 0.806 - 1.15 ) | 1.13 ( 0.939 - 1.3 ) |
| SM (OH) C14:1 | 4.21 ( 3.4 - 4.86 ) | 5.17 ( 4.48 - 6.01 ) | 4.84 ( 4.05 - 5.6 ) | 4.77 ( 4.18 - 5.4 ) | 4.14 ( 3.61 - 4.95 ) | 4.05 ( 3.4 - 4.54 ) |
| SM (OH) C16:1 | 2.14 ( 1.82 - 2.55 ) | 2.77 ( 2.39 - 3.23 ) | 2.58 ( 2.16 - 2.97 ) | 2.71 ( 2.3 - 3.04 ) | 2.19 ( 1.88 - 2.57 ) | 2.19 ( 1.88 - 2.5 ) |
| SM (OH) C22:1 | 6.74 ( 5.59 - 7.98 ) | 7.29 ( 6.24 - 8.5 ) | 7.38 ( 6.22 - 8.91 ) | 6.54 ( 5.6 - 7.85 ) | 8.22 ( 6.95 - 9.55 ) | 6.97 ( 5.92 - 8.32 ) |
| SM (OH) C22:2 | 5.48 ( 4.46 - 6.38 ) | 6.2 ( 5.2 - 7.15 ) | 5.66 ( 4.74 - 6.95 ) | 5.87 ( 5.02 - 6.98 ) | 5.67 ( 4.8 - 6.62 ) | 5.27 ( 4.34 - 6.14 ) |
| SM (OH) C24:1 | 0.542 ( 0.452 - 0.65 ) | 0.587 ( 0.487 - 0.71 ) | 0.584 ( 0.473 - 0.71 ) | 0.577 ( 0.474 - 0.672 ) | 0.608 ( 0.528 - 0.697 ) | 0.534 ( 0.434 - 0.64 ) |
| SM C16:0 | 89.2 ( 78.3 - 102 ) | 92.5 ( 83.2 - 102 ) | 91 ( 83.1 - 102 ) | 87.8 ( 80.6 - 97.7 ) | 95.7 ( 84.7 - 106 ) | 92.2 ( 80.6 - 102 ) |
| SM C16:1 | 11 ( 9.57 - 12.6 ) | 12.1 ( 10.7 - 13.6 ) | 11.1 ( 9.67 - 12.8 ) | 11 ( 9.92 - 12.5 ) | 11.7 ( 10.4 - 13.4 ) | 12 ( 10.6 - 13.2 ) |
| SM C18:0 | 15.1 ( 13.1 - 17.8 ) | 17.2 ( 15.3 - 19.9 ) | 16.4 ( 14.2 - 19 ) | 16.8 ( 14.4 - 19.6 ) | 16.6 ( 14.4 - 18.9 ) | 16.2 ( 13.1 - 18.5 ) |
| SM C18:1 | 7.16 ( 6.12 - 8.16 ) | 8.47 ( 7.55 - 9.62 ) | 7.77 ( 6.87 - 9.12 ) | 7.87 ( 6.92 - 9.27 ) | 7.77 ( 6.68 - 8.9 ) | 8.11 ( 6.86 - 9.07 ) |
| SM C20:2 | 0.304 ( 0.248 - 0.362 ) | 0.317 ( 0.264 - 0.373 ) | 0.334 ( 0.292 - 0.4 ) | 0.325 ( 0.28 - 0.388 ) | 0.325 ( 0.269 - 0.384 ) | 0.346 ( 0.286 - 0.42 ) |
| SM C24:0 | 10.5 ( 8.8 - 12.2 ) | 10.1 ( 8.62 - 12.2 ) | 10.6 ( 9.09 - 12.5 ) | 9.81 ( 8.32 - 11.5 ) | 11.2 ( 9.64 - 12.8 ) | 10.6 ( 8.95 - 12.6 ) |
| SM C24:1 | 22 ( 17.3 - 25.7 ) | 21.3 ( 18.3 - 24.2 ) | 20.9 ( 17.6 - 24.6 ) | 21.1 ( 18.5 - 26.1 ) | 20.2 ( 17.1 - 23.4 ) | 19.6 ( 15.8 - 23.2 ) |
| SM C26:0 | 0.076 ( 0.0605 - 0.09 ) | 0.079 ( 0.065 - 0.097 ) | 0.081 ( 0.065 - 0.101 ) | 0.088 ( 0.072 - 0.107 ) | 0.084 ( 0.067 - 0.1 ) | 0.077 ( 0.055 - 0.094 ) |
| SM C26:1 | 0.135 ( 0.114 - 0.168 ) | 0.145 ( 0.118 - 0.169 ) | 0.148 ( 0.119 - 0.18 ) | 0.178 ( 0.14 - 0.213 ) | 0.138 ( 0.11 - 0.164 ) | 0.132 ( 0.109 - 0.162 ) |
| H1 | 3880 ( 3530 - 4200 ) | 4200 ( 3910 - 4630 ) | 4080 ( 3840 - 4380 ) | 4010 ( 3740 - 4280 ) | 4100 ( 3820 - 4390 ) | 3990 ( 3710 - 4340 ) |

## Supplementary Table 6 Metabolites associated with age

| metabolite | effect size (SD/ year) | lower CI | upper CI | p-value | $I^2$ |
|---|---|---|---|---|---|
| creatinine (urine) | 0.39 | 0.26 | 0.53 | 4.4E-09 | 0% |
| Creatinine (serum) | 0.30 | 0.17 | 0.43 | 7.3E-06 | 23% |

## Supplementary Table 7 Metabolites associated with sex

| metabolite | effect size (SD) | lower CI | upper CI | p-value | $I^2$ |
|---|---|---|---|---|---|
| isoleucine (urine) | -0.24 | -0.37 | -0.12 | 1.1E-04 | 59% |
| 5-oxoproline (urine) | 0.23 | 0.11 | 0.36 | 2.3E-04 | 0% |
| tyrosine (urine) | 0.43 | 0.31 | 0.55 | 3.7E-12 | 9% |
| C10 | -0.23 | -0.35 | -0.11 | 2.6E-04 | 29% |
| C12 | -0.29 | -0.41 | -0.17 | 1.8E-06 | 27% |
| C14:1 | -0.34 | -0.46 | -0.22 | 5.8E-08 | 19% |
| C14:1-OH | -0.22 | -0.34 | -0.10 | 2.6E-04 | 19% |
| C14:2 | -0.24 | -0.36 | -0.12 | 7.9E-05 | 17% |
| C16:1 | -0.26 | -0.38 | -0.14 | 3.0E-05 | 15% |
| Lys | -0.24 | -0.35 | -0.12 | 1.1E-04 | 53% |
| Orn | -0.35 | -0.47 | -0.23 | 1.4E-08 | 18% |
| Ser | -0.26 | -0.39 | -0.14 | 2.1E-05 | 5% |
| Putrescine | -0.21 | -0.33 | -0.10 | 2.8E-04 | 55% |
| Serotonin | 0.32 | 0.20 | 0.44 | 1.8E-07 | 49% |
| SM C16:1 | -0.35 | -0.46 | -0.24 | 3.2E-10 | 0% |
| SM C18:0 | -0.22 | -0.33 | -0.11 | 9.2E-05 | 0% |
| SM C18:1 | -0.35 | -0.46 | -0.24 | 1.8E-10 | 0% |
| H1 | 0.23 | 0.11 | 0.35 | 2.4E-04 | 8% |

Metabolites found higher in male children are shown as positive and metabolites found higher in female children are shown as negative

## Supplementary Table 8 Metabolites associated with z-BMI score

| metabolite | effect size (SD/ unit z-score) | lower CI | upper CI | p-value | $I^2$ |
|---|---|---|---|---|---|
| valine (urine) | 0.09 | 0.04 | 0.15 | 4.1E-04 | 0% |
| 4-deoxyerythronic acid (urine) | 0.21 | 0.16 | 0.26 | 8.1E-16 | 40% |
| *p*-cresol sulfate (urine) | -0.10 | -0.16 | -0.05 | 1.1E-04 | 63% |
| pantothenate (urine) | -0.12 | -0.17 | -0.07 | 2.0E-06 | 13% |
| C0 | 0.18 | 0.13 | 0.24 | 1.4E-12 | 0% |
| C18 | -0.13 | -0.18 | -0.08 | 1.1E-06 | 14% |
| C3 | 0.15 | 0.10 | 0.20 | 7.6E-10 | 0% |
| C5 | 0.13 | 0.08 | 0.18 | 1.0E-06 | 0% |
| Asp | 0.10 | 0.05 | 0.15 | 1.5E-04 | 20% |
| Glu | 0.22 | 0.17 | 0.27 | 3.3E-17 | 0% |
| Leu | 0.11 | 0.06 | 0.16 | 4.3E-05 | 0% |
| Lys | 0.10 | 0.05 | 0.15 | 2.1E-04 | 0% |
| Phe | 0.12 | 0.07 | 0.17 | 3.4E-06 | 23% |
| Pro | 0.10 | 0.05 | 0.15 | 1.2E-04 | 0% |
| Val | 0.12 | 0.07 | 0.18 | 2.5E-06 | 0% |
| ADMA | 0.09 | 0.04 | 0.15 | 2.7E-04 | 0% |
| alpha-AAA | 0.10 | 0.05 | 0.15 | 8.7E-05 | 0% |
| Kynurenine | 0.10 | 0.05 | 0.15 | 1.1E-04 | 36% |
| lysoPC a C14:0 | 0.09 | 0.04 | 0.14 | 2.6E-04 | 0% |
| lysoPC a C16:1 | 0.14 | 0.09 | 0.19 | 1.1E-07 | 0% |
| lysoPC a C18:1 | -0.09 | -0.14 | -0.05 | 1.8E-04 | 0% |
| lysoPC a C18:2 | -0.12 | -0.17 | -0.07 | 4.9E-06 | 0% |
| PC aa C32:1 | 0.11 | 0.06 | 0.16 | 1.4E-05 | 0% |
| PC aa C32:3 | 0.10 | 0.05 | 0.15 | 5.9E-05 | 0% |
| PC aa C34:4 | 0.14 | 0.08 | 0.19 | 2.3E-07 | 0% |
| PC aa C36:5 | 0.10 | 0.05 | 0.15 | 1.5E-04 | 0% |
| PC aa C36:6 | 0.10 | 0.04 | 0.15 | 2.6E-04 | 0% |
| PC aa C38:1 | -0.10 | -0.15 | -0.05 | 8.2E-05 | 38% |
| PC aa C38:3 | 0.20 | 0.15 | 0.25 | 5.6E-16 | 0% |
| PC aa C38:4 | 0.14 | 0.08 | 0.19 | 1.5E-07 | 0% |
| PC aa C40:6 | 0.10 | 0.05 | 0.15 | 1.2E-04 | 0% |
| PC ae C34:0 | -0.10 | -0.14 | -0.05 | 1.8E-04 | 0% |
| PC ae C34:1 | -0.09 | -0.14 | -0.04 | 2.2E-04 | 0% |
| PC ae C36:0 | -0.10 | -0.15 | -0.05 | 2.4E-05 | 0% |
| PC ae C36:2 | -0.12 | -0.17 | -0.07 | 2.6E-06 | 0% |
| PC ae C38:2 | -0.10 | -0.15 | -0.05 | 5.6E-05 | 3% |
| PC ae C40:4 | -0.11 | -0.16 | -0.06 | 2.4E-05 | 23% |
| PC ae C40:5 | -0.10 | -0.15 | -0.05 | 1.1E-04 | 12% |
| PC ae C40:6 | -0.10 | -0.15 | -0.05 | 1.5E-04 | 0% |
| PC ae C42:3 | -0.11 | -0.16 | -0.06 | 1.6E-05 | 0% |
| PC ae C42:4 | -0.14 | -0.19 | -0.09 | 1.7E-07 | 0% |
| PC ae C44:4 | -0.11 | -0.16 | -0.05 | 5.7E-05 | 21% |
| SM C16:0 | -0.10 | -0.14 | -0.05 | 7.3E-05 | 18% |
| SM C16:1 | 0.16 | 0.11 | 0.21 | 1.3E-11 | 0% |
| SM C18:1 | 0.16 | 0.11 | 0.20 | 6.0E-11 | 0% |

## Supplementary Table 9 Metabolites associated with dietary intake

| metabolite-diet pair | effect size (SD/ times per week) | lower CI | upper CI | p-value | $I^2$ |
|---|---|---|---|---|---|
| creatine (urine) with meat | 0.025 | 0.012 | 0.039 | 2.9E-04 | 0% |
| pantothenate (urine) with dairy | 0.009 | 0.004 | 0.015 | 7.3E-04 | 39% |
| acetate (urine) with potatoes | 0.045 | 0.023 | 0.068 | 1.0E-04 | 0% |
| hippurate (urine) with vegetables | 0.021 | 0.011 | 0.031 | 2.0E-05 | 4% |
| leucine (urine) with fruits | -0.014 | -0.022 | -0.006 | 5.3E-04 | 0% |
| alanine (urine) with fruits | -0.014 | -0.022 | -0.006 | 7.7E-04 | 28% |
| glutamine (urine) with fruits | -0.013 | -0.021 | -0.005 | 9.3E-04 | 0% |
| *scyllo*-inositol (urine) with fruits | 0.014 | 0.007 | 0.021 | 9.0E-05 | 61% |
| hippurate (urine) with fruits | 0.026 | 0.018 | 0.034 | 4.4E-11 | 52% |
| proline betaine (urine) with fruits | 0.017 | 0.009 | 0.025 | 3.9E-05 | 0% |
| *N*-methylnicotinic acid (urine) with fruits | 0.017 | 0.009 | 0.025 | 4.1E-05 | 61% |
| 3-hydroxybutyrate/ 3-aminoisobutyrate (urine) with beverages | -0.049 | -0.067 | -0.030 | 2.2E-07 | 48% |
| PC ae C36:3 with meat | 0.024 | 0.011 | 0.037 | 2.1E-04 | 0% |
| PC ae C36:4 with meat | 0.031 | 0.018 | 0.044 | 3.5E-06 | 5% |
| PC ae C36:5 with meat | 0.026 | 0.013 | 0.040 | 1.1E-04 | 0% |
| PC ae C38:5 with meat | 0.027 | 0.014 | 0.040 | 5.6E-05 | 23% |
| PC aa C36:0 with fish | 0.091 | 0.063 | 0.119 | 9.6E-11 | 56% |
| PC aa C36:5 with fish | 0.062 | 0.034 | 0.090 | 1.5E-05 | 44% |
| PC aa C36:6 with fish | 0.086 | 0.058 | 0.114 | 1.2E-09 | 0% |
| PC aa C38:0 with fish | 0.107 | 0.080 | 0.134 | 1.3E-14 | 74% |
| PC aa C38:6 with fish | 0.112 | 0.084 | 0.140 | 1.9E-15 | 59% |
| PC aa C40:1 with fish | 0.053 | 0.026 | 0.081 | 1.5E-04 | 0% |
| PC aa C40:4 with fish | -0.057 | -0.084 | -0.030 | 3.4E-05 | 21% |
| PC aa C40:6 with fish | 0.099 | 0.071 | 0.127 | 2.5E-12 | 51% |
| PC aa C42:2 with fish | 0.057 | 0.030 | 0.084 | 4.6E-05 | 13% |
| PC ae C38:0 with fish | 0.084 | 0.057 | 0.112 | 1.5E-09 | 40% |
| PC ae C38:6 with fish | 0.074 | 0.046 | 0.102 | 2.3E-07 | 57% |
| PC ae C40:6 with fish | 0.086 | 0.058 | 0.113 | 1.4E-09 | 34% |
| PC aa C28:1 with dairy | 0.015 | 0.010 | 0.021 | 2.6E-08 | 59% |
| PC aa C30:0 with dairy | 0.012 | 0.007 | 0.017 | 1.2E-05 | 70% |
| PC aa C38:0 with dairy | -0.013 | -0.018 | -0.007 | 2.9E-06 | 0% |
| PC ae C30:0 with dairy | 0.015 | 0.010 | 0.020 | 2.2E-08 | 74% |
| PC ae C38:6 with dairy | -0.010 | -0.016 | -0.005 | 2.7E-04 | 0% |
| SM (OH) C14:1 with dairy | 0.013 | 0.007 | 0.018 | 2.7E-06 | 71% |
| PC ae C30:0 with potatoes | -0.042 | -0.064 | -0.020 | 1.7E-04 | 0% |
| PC ae C34:0 with potatoes | -0.049 | -0.071 | -0.027 | 1.2E-05 | 29% |
| SM (OH) C14:1 with potatoes | -0.049 | -0.070 | -0.027 | 1.2E-05 | 52% |
| Ac-Orn with fruits | 0.016 | 0.008 | 0.024 | 5.7E-05 | 0% |
| PC aa C38:0 with sweets | -0.021 | -0.031 | -0.011 | 2.2E-05 | 0% |
| PC aa C38:6 with sweets | -0.020 | -0.030 | -0.010 | 8.6E-05 | 0% |
| PC ae C38:5 with sweets | -0.020 | -0.030 | -0.011 | 4.5E-05 | 0% |
| PC ae C38:6 with sweets | -0.020 | -0.030 | -0.010 | 1.2E-04 | 0% |
| PC ae C40:6 with sweets | -0.022 | -0.032 | -0.012 | 1.4E-05 | 0% |
| lysoPC a C17:0 with bakery products | -0.026 | -0.039 | -0.013 | 5.7E-05 | 56% |
| PC aa C36:6 with bakery products | -0.028 | -0.041 | -0.015 | 2.7E-05 | 0% |
| PC aa C38:0 with bakery products | -0.027 | -0.040 | -0.014 | 3.3E-05 | 52% |
| PC aa C38:6 with bakery products | -0.028 | -0.041 | -0.014 | 3.5E-05 | 52% |
| PC aa C40:6 with bakery products | -0.027 | -0.040 | -0.015 | 2.9E-05 | 41% |
| PC ae C38:0 with bakery products | -0.030 | -0.043 | -0.017 | 3.9E-06 | 15% |
| PC ae C38:6 with bakery products | -0.025 | -0.038 | -0.012 | 1.3E-04 | 14% |
| PC ae C40:2 with bakery products | -0.027 | -0.040 | -0.014 | 4.3E-05 | 53% |
| PC ae C40:6 with bakery products | -0.026 | -0.039 | -0.013 | 6.6E-05 | 36% |
| SM (OH) C14:1 with bakery products | -0.027 | -0.040 | -0.015 | 2.4E-05 | 27% |
| SM (OH) C16:1 with bakery products | -0.031 | -0.043 | -0.018 | 9.7E-07 | 43% |
| C5:1 with beverages | -0.032 | -0.050 | -0.015 | 2.7E-04 | 0% |
| C6:1 with beverages | -0.030 | -0.046 | -0.014 | 2.6E-04 | 15% |
| SM (OH) C16:1 with beverages | -0.032 | -0.050 | -0.015 | 2.3E-04 | 0% |

## Supplementary Table 10 Variance decomposition analysis of urine metabolites (% variance explained)

| | analytical | pre-analytical | demographic | dietary | cohort | residual |
|---|---|---|---|---|---|---|
| creatinine | 2.5 | 1.1 | 7.0 | 1.8 | 2.0 | 85.7 |
| leucine | 1.5 | 0.4 | 1.4 | 3.1 | 2.3 | 91.4 |
| isoleucine | 1.3 | 0.0 | 0.5 | 0.6 | 0.5 | 97.1 |
| valine | 1.5 | 0.6 | 2.7 | 3.1 | 1.7 | 90.4 |
| 3-hydroxyisobutyrate | 0.8 | 1.3 | 2.2 | 1.3 | 1.0 | 93.5 |
| 4-deoxyerythronic acid | 1.4 | 0.8 | 9.0 | 2.5 | 3.0 | 83.4 |
| 4-deoxythreonic acid | 1.5 | 1.5 | 3.8 | 1.1 | 1.4 | 90.7 |
| threonine/ lactate | 1.9 | 1.0 | 0.6 | 1.5 | 0.9 | 94.1 |
| 2-hydroxyisobutyrate | 2.0 | 1.6 | 1.0 | 2.9 | 1.2 | 91.3 |
| alanine | 1.2 | 1.5 | 0.6 | 2.3 | 1.4 | 93.1 |
| lysine | 1.1 | 0.0 | 0.7 | 1.7 | 1.0 | 95.5 |
| acetate | 3.1 | 0.7 | 1.4 | 2.5 | 1.0 | 91.2 |
| *p*-cresol sulfate | 1.9 | 0.2 | 0.9 | 1.3 | 1.5 | 94.2 |
| succinate | 1.8 | 0.3 | 2.5 | 1.1 | 1.0 | 93.3 |
| glutamine | 2.2 | 0.3 | 0.4 | 1.1 | 0.2 | 95.9 |
| citrate | 1.9 | 2.4 | 2.8 | 1.6 | 3.9 | 87.5 |
| dimethylamine | 1.1 | 1.4 | 0.5 | 1.6 | 0.8 | 94.7 |
| trimethylamine | 1.2 | 0.2 | 1.1 | 0.9 | 0.9 | 95.7 |
| carnitine/ choline | 1.3 | 0.5 | 2.9 | 2.2 | 1.0 | 92.2 |
| trimethylamine *N*-oxide | 1.3 | 1.0 | 1.0 | 1.1 | 0.5 | 95.1 |
| *scyllo*-inositol | 15.8 | 0.1 | 0.8 | 1.5 | 1.4 | 80.4 |
| taurine | 3.7 | 0.4 | 1.9 | 3.1 | 1.4 | 89.6 |
| glycine | 1.7 | 1.2 | 0.5 | 1.6 | 4.1 | 90.8 |
| creatine | 1.5 | 1.2 | 1.1 | 2.6 | 3.0 | 90.6 |
| hippurate | 1.6 | 1.6 | 3.5 | 7.8 | 7.4 | 78.0 |
| formate | 1.0 | 0.2 | 3.6 | 1.0 | 0.8 | 93.5 |
| pantothenate | 1.0 | 0.2 | 6.7 | 2.8 | 0.7 | 88.7 |
| 3-hydroxybutyrate/ 3-aminoisobutyrate | 1.5 | 1.6 | 0.2 | 3.7 | 2.1 | 90.9 |
| 3-hydroxyisovalerate | 1.1 | 1.3 | 2.8 | 1.8 | 1.1 | 91.9 |
| *N*-acetyl-neuraminic acid | 2.6 | 2.4 | 0.7 | 2.3 | 1.1 | 90.8 |
| acetone | 3.2 | 1.1 | 3.3 | 1.2 | 4.0 | 87.2 |
| 5-oxoproline | 1.3 | 0.4 | 1.2 | 1.4 | 1.3 | 94.4 |
| 3-aminoisobutyrate | 2.1 | 0.2 | 0.6 | 2.7 | 1.4 | 93.0 |
| proline betaine | 0.5 | 0.5 | 0.3 | 2.7 | 1.7 | 94.3 |
| glucose | 1.0 | 1.1 | 0.7 | 1.1 | 0.6 | 95.6 |
| sucrose | 2.2 | 0.4 | 2.5 | 2.3 | 5.5 | 87.1 |
| urea | 2.1 | 0.3 | 1.8 | 2.9 | 1.4 | 91.4 |
| *N*-methyl-2-pyridone-5-carboxamide | 1.9 | 0.2 | 1.0 | 0.9 | 1.8 | 94.1 |
| *p*-hydroxyphenylacetate | 1.5 | 1.8 | 0.5 | 1.7 | 4.2 | 90.4 |
| tyrosine | 2.1 | 0.6 | 5.0 | 0.6 | 2.0 | 89.8 |
| 3-Indoxylsulfate | 1.2 | 0.3 | 1.3 | 0.8 | 0.2 | 96.2 |
| *N*-methylpicolinic acid | 1.3 | 0.1 | 0.3 | 0.7 | 1.6 | 96.0 |
| *N*-methylnicotinic acid | 0.4 | 1.2 | 1.5 | 4.1 | 0.1 | 92.7 |
| *N*-methyl nicotinamide | 1.4 | 5.5 | 1.3 | 1.2 | 1.1 | 89.6 |

**Supplementary Table 11 Variance decomposition analysis of serum metabolites (% variance explained)**

| | analytical | pre-analytical | demographic | dietary | cohort | residual |
|---|---|---|---|---|---|---|
| C0 | 3.6 | 0.7 | 6.9 | 0.4 | 0.3 | 88.0 |
| C10 | 3.3 | 1.0 | 5.8 | 2.0 | 2.6 | 85.3 |
| C10:1 | 3.2 | 1.2 | 7.4 | 2.5 | 5.7 | 80.0 |
| C10:2 | 6.2 | 0.0 | 4.6 | 2.8 | 6.5 | 80.0 |
| C12 | 3.7 | 1.2 | 8.1 | 1.8 | 3.0 | 82.3 |
| C12-DC | 35.8 | 0.0 | 0.3 | 0.6 | 0.1 | 63.2 |
| C12:1 | 5.0 | 1.3 | 6.4 | 1.7 | 2.3 | 83.2 |
| C14 | 42.6 | 0.4 | 2.6 | 0.9 | 1.4 | 52.0 |
| C14:1 | 2.2 | 2.6 | 7.0 | 1.4 | 1.3 | 85.5 |
| C14:1-OH | 6.7 | 0.6 | 4.1 | 1.2 | 1.7 | 85.7 |
| C14:2 | 2.6 | 2.0 | 6.2 | 2.3 | 3.5 | 83.3 |
| C14:2-OH | 57.3 | 0.0 | 0.4 | 0.5 | 0.5 | 41.3 |
| C16 | 5.2 | 1.6 | 7.0 | 2.2 | 3.9 | 80.0 |
| C16-OH | 83.0 | 0.0 | 0.1 | 0.2 | 0.0 | 16.7 |
| C16:1 | 3.0 | 2.8 | 4.9 | 1.3 | 0.8 | 87.2 |
| C16:1-OH | 17.8 | 0.7 | 3.1 | 1.1 | 1.3 | 75.9 |
| C16:2 | 28.3 | 0.9 | 2.8 | 0.8 | 0.4 | 66.7 |
| C16:2-OH | 22.6 | 0.2 | 3.2 | 0.9 | 1.1 | 72.0 |
| C18 | 6.1 | 0.4 | 5.2 | 2.3 | 0.6 | 85.3 |
| C18:1 | 4.2 | 4.8 | 6.4 | 2.3 | 3.0 | 79.3 |
| C18:2 | 4.3 | 2.1 | 9.5 | 3.3 | 6.9 | 73.8 |
| C2 | 1.1 | 3.4 | 5.2 | 1.3 | 2.4 | 86.5 |
| C3 | 16.7 | 1.4 | 4.7 | 0.8 | 2.3 | 74.1 |
| C3-DC (C4-OH) | 16.6 | 0.5 | 3.8 | 2.3 | 1.1 | 75.7 |
| C3-OH | 68.0 | 0.0 | 0.1 | 0.4 | 0.2 | 31.4 |
| C4 | 14.7 | 0.5 | 1.3 | 1.6 | 1.6 | 80.4 |
| C4:1 | 64.0 | 0.0 | 0.2 | 0.6 | 0.3 | 34.8 |
| C6 (C4:1-DC) | 7.4 | 1.1 | 4.6 | 1.7 | 2.5 | 82.8 |
| C5 | 2.6 | 1.3 | 4.4 | 2.5 | 1.1 | 88.1 |
| C5-M-DC | 55.4 | 0.1 | 0.9 | 0.7 | 0.3 | 42.7 |
| C5-OH (C3-DC-M) | 17.4 | 0.6 | 1.6 | 1.7 | 0.4 | 78.4 |
| C5:1 | 10.6 | 0.1 | 0.7 | 3.2 | 0.7 | 84.7 |
| C5:1-DC | 59.3 | 0.3 | 0.2 | 0.7 | 0.2 | 39.3 |
| C5-DC (C6-OH) | 34.6 | 0.3 | 1.5 | 1.3 | 0.4 | 61.9 |
| C6:1 | 24.0 | 0.1 | 3.1 | 3.8 | 1.8 | 67.2 |
| C7-DC | 39.3 | 0.6 | 2.4 | 0.6 | 0.6 | 56.6 |
| C8 | 9.8 | 1.0 | 4.6 | 1.6 | 2.1 | 81.0 |
| C9 | 14.5 | 0.0 | 2.6 | 6.4 | 7.0 | 69.5 |
| Ala | 3.9 | 2.0 | 2.6 | 2.1 | 2.3 | 87.1 |
| Arg | 4.8 | 0.5 | 0.8 | 1.9 | 4.4 | 87.7 |
| Asn | 4.7 | 0.8 | 1.3 | 2.4 | 4.6 | 86.2 |
| Asp | 5.6 | 4.3 | 13.5 | 4.3 | 11.3 | 61.1 |
| Cit | 6.5 | 0.0 | 3.8 | 1.6 | 4.3 | 83.8 |
| Gln | 5.4 | 0.0 | 3.2 | 2.5 | 7.6 | 81.2 |
| Glu | 2.1 | 0.5 | 23.8 | 2.8 | 5.4 | 65.5 |
| Gly | 6.2 | 0.3 | 2.5 | 2.4 | 4.8 | 83.8 |
| His | 9.2 | 0.9 | 0.5 | 1.7 | 1.0 | 86.7 |
| Ile | 1.9 | 0.3 | 3.8 | 4.0 | 5.6 | 84.4 |
| Leu | 2.1 | 0.3 | 3.5 | 4.3 | 4.3 | 85.4 |
| Lys | 6.0 | 1.1 | 5.4 | 1.6 | 1.9 | 84.0 |
| Met | 11.5 | 0.8 | 0.9 | 1.5 | 1.6 | 83.7 |
| Orn | 4.9 | 0.4 | 4.7 | 2.5 | 4.8 | 82.7 |
| Phe | 4.7 | 1.0 | 2.9 | 4.5 | 4.2 | 82.6 |
| Pro | 2.9 | 1.5 | 1.9 | 0.6 | 2.1 | 91.1 |
| Ser | 7.0 | 0.6 | 5.4 | 0.9 | 2.9 | 83.2 |
| Thr | 4.4 | 0.7 | 5.3 | 1.5 | 3.5 | 84.7 |
| Trp | 9.4 | 0.9 | 3.0 | 2.7 | 3.2 | 80.9 |
| Tyr | 2.4 | 0.4 | 2.5 | 2.4 | 3.4 | 88.8 |
| Val | 3.3 | 0.3 | 5.1 | 4.0 | 4.2 | 83.2 |
| Ac-Orn | 3.6 | 0.1 | 2.0 | 7.4 | 12.6 | 74.3 |
| ADMA | 7.2 | 0.3 | 5.3 | 1.1 | 3.2 | 82.9 |
| alpha-AAA | 12.2 | 0.4 | 3.6 | 3.3 | 3.5 | 77.1 |
| Creatinine | 3.8 | 0.6 | 14.1 | 2.0 | 1.7 | 77.7 |
| Kynurenine | 4.6 | 0.6 | 1.5 | 1.2 | 1.4 | 90.7 |
| Met-SO | 6.9 | 0.3 | 17.3 | 2.7 | 4.2 | 68.6 |
| Putrescine | 14.1 | 0.5 | 1.9 | 1.0 | 1.1 | 81.5 |
| SDMA | 59.7 | 0.1 | 1.3 | 0.4 | 0.5 | 37.9 |
| Serotonin | 2.6 | 1.3 | 4.9 | 1.5 | 5.2 | 84.5 |
| Spermidine | 29.6 | 2.4 | 0.9 | 1.0 | 1.7 | 64.4 |
| Spermine | 51.2 | 0.3 | 0.3 | 0.3 | 0.8 | 47.0 |
| t4-OH-Pro | 5.6 | 0.1 | 1.9 | 2.6 | 0.4 | 89.4 |
| Taurine | 2.5 | 3.4 | 8.9 | 4.4 | 13.9 | 66.9 |
| total DMA | 32.5 | 0.1 | 4.7 | 0.9 | 3.9 | 58.0 |
| lysoPC a C14:0 | 17.5 | 0.8 | 1.6 | 3.4 | 2.5 | 74.2 |
| lysoPC a C16:0 | 13.2 | 0.3 | 1.0 | 2.9 | 3.8 | 78.7 |
| lysoPC a C16:1 | 8.3 | 0.5 | 2.8 | 2.3 | 4.4 | 81.7 |

| | | | | | | |
|---|---|---|---|---|---|---|
| lysoPC a C17:0 | 9.5 | 1.6 | 3.1 | 5.6 | 5.0 | 75.1 |
| lysoPC a C18:0 | 12.6 | 0.2 | 0.3 | 2.0 | 2.3 | 82.6 |
| lysoPC a C18:1 | 8.3 | 0.3 | 3.4 | 5.2 | 9.1 | 73.8 |
| lysoPC a C18:2 | 6.0 | 0.6 | 3.1 | 3.5 | 6.5 | 80.2 |
| lysoPC a C20:3 | 5.2 | 0.1 | 3.0 | 9.6 | 8.8 | 73.4 |
| lysoPC a C20:4 | 8.0 | 0.0 | 2.5 | 6.0 | 7.6 | 75.9 |
| lysoPC a C24:0 | 19.8 | 0.1 | 0.9 | 0.8 | 1.7 | 76.8 |
| lysoPC a C26:0 | 20.5 | 0.1 | 0.2 | 1.1 | 0.3 | 77.9 |
| lysoPC a C26:1 | 25.5 | 0.0 | 0.3 | 0.6 | 0.4 | 73.1 |
| lysoPC a C28:0 | 18.6 | 0.1 | 0.2 | 1.2 | 0.3 | 79.6 |
| lysoPC a C28:1 | 20.4 | 0.2 | 0.7 | 1.1 | 1.3 | 76.4 |
| PC aa C24:0 | 17.7 | 0.0 | 0.4 | 0.6 | 0.1 | 81.2 |
| PC aa C28:1 | 7.8 | 0.4 | 3.5 | 6.9 | 4.1 | 77.3 |
| PC aa C30:0 | 5.4 | 0.2 | 1.1 | 4.8 | 5.1 | 83.4 |
| PC aa C30:2 | 26.5 | 0.2 | 0.2 | 0.6 | 0.0 | 72.4 |
| PC aa C32:0 | 17.9 | 0.1 | 1.8 | 1.1 | 4.6 | 74.6 |
| PC aa C32:1 | 6.3 | 0.1 | 2.0 | 3.4 | 7.1 | 81.1 |
| PC aa C32:2 | 6.5 | 0.2 | 2.1 | 2.0 | 1.1 | 88.0 |
| PC aa C32:3 | 17.6 | 0.2 | 2.9 | 4.9 | 4.7 | 69.6 |
| PC aa C34:1 | 12.9 | 0.1 | 1.0 | 2.6 | 6.0 | 77.3 |
| PC aa C34:2 | 15.4 | 0.1 | 2.3 | 2.8 | 4.6 | 74.9 |
| PC aa C34:3 | 8.4 | 0.4 | 2.7 | 5.1 | 7.5 | 75.9 |
| PC aa C34:4 | 6.1 | 0.2 | 6.2 | 1.7 | 0.6 | 85.3 |
| PC aa C36:0 | 7.7 | 0.3 | 5.3 | 9.1 | 3.9 | 73.7 |
| PC aa C36:1 | 8.3 | 0.3 | 1.3 | 1.8 | 4.7 | 83.5 |
| PC aa C36:2 | 13.3 | 0.1 | 0.4 | 1.5 | 2.1 | 82.6 |
| PC aa C36:3 | 13.0 | 0.2 | 1.1 | 4.6 | 3.2 | 77.9 |
| PC aa C36:4 | 11.3 | 0.0 | 2.2 | 3.0 | 4.9 | 78.5 |
| PC aa C36:5 | 3.3 | 0.3 | 3.1 | 18.8 | 19.8 | 54.6 |
| PC aa C36:6 | 4.5 | 0.3 | 8.3 | 15.4 | 12.3 | 59.3 |
| PC aa C38:0 | 5.9 | 0.5 | 7.2 | 14.7 | 5.6 | 66.0 |
| PC aa C38:1 | 4.7 | 0.4 | 3.7 | 8.8 | 6.7 | 75.7 |
| PC aa C38:3 | 8.0 | 0.3 | 8.6 | 3.5 | 1.7 | 77.8 |
| PC aa C38:4 | 8.1 | 0.0 | 5.2 | 2.5 | 3.5 | 80.6 |
| PC aa C38:5 | 7.4 | 0.2 | 1.2 | 6.7 | 6.4 | 78.0 |
| PC aa C38:6 | 4.3 | 0.6 | 6.7 | 15.5 | 9.6 | 63.3 |
| PC aa C40:1 | 9.2 | 0.9 | 2.2 | 8.9 | 4.5 | 74.3 |
| PC aa C40:2 | 8.7 | 0.4 | 1.7 | 4.1 | 1.8 | 83.3 |
| PC aa C40:3 | 15.2 | 0.5 | 1.6 | 5.4 | 3.9 | 73.5 |
| PC aa C40:4 | 6.1 | 0.1 | 3.6 | 4.0 | 1.7 | 84.4 |
| PC aa C40:5 | 5.2 | 0.0 | 1.6 | 3.9 | 5.2 | 84.0 |
| PC aa C40:6 | 2.9 | 0.5 | 9.7 | 14.9 | 11.7 | 60.4 |
| PC aa C42:0 | 5.2 | 0.5 | 3.2 | 7.0 | 4.2 | 80.1 |
| PC aa C42:1 | 6.5 | 0.6 | 2.1 | 6.4 | 2.6 | 81.8 |
| PC aa C42:2 | 8.4 | 0.4 | 2.9 | 6.2 | 2.5 | 79.7 |
| PC aa C42:4 | 10.5 | 0.1 | 0.8 | 0.8 | 0.3 | 87.6 |
| PC aa C42:5 | 8.0 | 0.2 | 3.1 | 11.8 | 15.0 | 62.0 |
| PC aa C42:6 | 6.2 | 0.6 | 3.4 | 14.9 | 18.6 | 56.3 |
| PC ae C30:0 | 9.8 | 0.9 | 3.3 | 6.1 | 8.3 | 71.7 |
| PC ae C30:1 | 26.4 | 0.2 | 0.9 | 0.6 | 0.5 | 71.4 |
| PC ae C30:2 | 18.0 | 0.5 | 2.7 | 1.3 | 1.6 | 75.9 |
| PC ae C32:1 | 19.4 | 0.0 | 3.2 | 0.8 | 2.7 | 73.9 |
| PC ae C32:2 | 23.2 | 0.2 | 5.9 | 2.3 | 1.9 | 66.4 |
| PC ae C34:0 | 9.6 | 0.2 | 3.9 | 6.1 | 6.8 | 73.4 |
| PC ae C34:1 | 17.4 | 0.1 | 3.2 | 1.4 | 3.8 | 74.2 |
| PC ae C34:2 | 12.4 | 0.1 | 2.7 | 1.9 | 4.6 | 78.3 |
| PC ae C34:3 | 12.9 | 0.1 | 0.7 | 1.6 | 2.2 | 82.5 |
| PC ae C36:0 | 18.4 | 0.7 | 3.4 | 3.2 | 4.7 | 69.7 |
| PC ae C36:1 | 11.5 | 0.2 | 1.7 | 5.8 | 6.6 | 74.2 |
| PC ae C36:2 | 11.7 | 0.8 | 2.5 | 3.8 | 2.4 | 78.9 |
| PC ae C36:3 | 13.0 | 0.0 | 3.9 | 2.7 | 2.4 | 77.9 |
| PC ae C36:4 | 8.4 | 0.0 | 7.9 | 5.9 | 8.3 | 69.5 |
| PC ae C36:5 | 8.8 | 0.0 | 4.1 | 3.1 | 4.1 | 79.9 |
| PC ae C38:0 | 6.4 | 0.5 | 5.3 | 18.4 | 13.4 | 55.9 |
| PC ae C38:1 | 7.7 | 0.2 | 1.5 | 1.8 | 2.7 | 86.1 |
| PC ae C38:2 | 10.5 | 0.3 | 2.0 | 2.1 | 0.3 | 84.8 |
| PC ae C38:3 | 9.6 | 0.4 | 0.9 | 2.6 | 1.1 | 85.5 |
| PC ae C38:4 | 9.9 | 0.2 | 5.9 | 2.2 | 3.3 | 78.5 |
| PC ae C38:5 | 9.6 | 0.0 | 6.8 | 4.7 | 4.1 | 74.8 |
| PC ae C38:6 | 6.3 | 0.3 | 7.5 | 8.9 | 3.8 | 73.2 |
| PC ae C40:1 | 10.8 | 0.2 | 3.8 | 6.1 | 1.9 | 77.1 |
| PC ae C40:2 | 5.2 | 0.4 | 1.9 | 13.4 | 15.2 | 63.9 |
| PC ae C40:3 | 9.1 | 0.3 | 0.9 | 1.5 | 1.4 | 86.8 |
| PC ae C40:4 | 10.4 | 0.1 | 2.8 | 1.2 | 1.3 | 84.1 |
| PC ae C40:5 | 8.2 | 0.3 | 3.1 | 1.3 | 0.5 | 86.7 |
| PC ae C40:6 | 4.9 | 0.8 | 7.0 | 12.9 | 10.0 | 64.4 |
| PC ae C42:0 | 14.6 | 0.8 | 1.5 | 10.5 | 7.3 | 65.3 |
| PC ae C42:1 | 14.7 | 0.2 | 1.1 | 1.8 | 1.1 | 81.2 |
| PC ae C42:2 | 8.2 | 0.6 | 1.9 | 6.5 | 7.5 | 75.3 |
| PC ae C42:3 | 10.3 | 1.1 | 2.8 | 4.6 | 3.2 | 77.8 |
| PC ae C42:4 | 8.5 | 0.2 | 3.0 | 0.7 | 0.3 | 87.4 |

| | | | | | | |
|---|---|---|---|---|---|---|
| PC ae C42:5 | 7.1 | 0.5 | 3.2 | 0.7 | 0.1 | 88.4 |
| PC ae C44:3 | 15.1 | 0.3 | 1.5 | 0.7 | 2.1 | 80.3 |
| PC ae C44:4 | 7.5 | 0.4 | 2.3 | 1.1 | 1.0 | 87.6 |
| PC ae C44:5 | 5.8 | 0.2 | 3.6 | 0.5 | 0.2 | 89.7 |
| PC ae C44:6 | 6.0 | 0.2 | 1.6 | 2.0 | 3.0 | 87.1 |
| SM (OH) C14:1 | 10.6 | 0.8 | 4.2 | 7.1 | 7.6 | 69.7 |
| SM (OH) C16:1 | 13.6 | 0.8 | 6.0 | 6.8 | 8.1 | 64.6 |
| SM (OH) C22:1 | 38.0 | 0.1 | 1.9 | 1.6 | 4.6 | 53.9 |
| SM (OH) C22:2 | 39.2 | 0.2 | 1.0 | 2.7 | 3.9 | 52.9 |
| SM (OH) C24:1 | 33.1 | 0.2 | 0.7 | 1.2 | 2.9 | 61.8 |
| SM C16:0 | 22.0 | 0.2 | 1.3 | 0.7 | 1.1 | 74.7 |
| SM C16:1 | 18.9 | 0.0 | 8.7 | 1.0 | 1.5 | 69.9 |
| SM C18:0 | 22.3 | 0.1 | 3.5 | 0.7 | 1.7 | 71.8 |
| SM C18:1 | 20.2 | 0.1 | 9.5 | 0.9 | 1.3 | 68.0 |
| SM C20:2 | 21.6 | 0.0 | 1.7 | 0.8 | 2.0 | 73.9 |
| SM C24:0 | 44.6 | 0.5 | 1.4 | 0.9 | 0.6 | 52.1 |
| SM C24:1 | 42.5 | 0.2 | 0.5 | 2.1 | 2.5 | 52.2 |
| SM C26:0 | 22.1 | 0.6 | 1.6 | 2.0 | 2.8 | 70.9 |
| SM C26:1 | 20.5 | 0.6 | 1.1 | 5.2 | 5.4 | 67.2 |
| H1 | 4.9 | 0.5 | 4.3 | 0.6 | 2.9 | 86.9 |

## Supplementary Table 12 Modeled results with Box-Cox transformation and QRILC imputation - metabolites associated with age

| metabolite | effect size (SD/ year) | lower CI | upper CI | p-value | $I^2$ |
|---|---|---|---|---|---|
| creatinine (urine) | 0.39 | 0.26 | 0.53 | 4.7E-09 | 0% |
| Creatinine (serum) | 0.30 | 0.17 | 0.43 | 4.0E-06 | 19% |

## Supplementary Table 13 Modeled results with Box-Cox transformation and QRILC imputation - metabolites associated with sex

| metabolite | effect size | lower CI | upper CI | p-value | $I^2$ |
|---|---|---|---|---|---|
| isoleucine (urine) | -0.28 | -0.41 | -0.16 | 6.2E-06 | 67% |
| glutamine (urine) | 0.21 | 0.09 | 0.34 | 6.9E-04 | 0% |
| citrate (urine) | -0.21 | -0.33 | -0.09 | 4.8E-04 | 21% |
| 5-oxoproline (urine) | 0.23 | 0.10 | 0.36 | 3.7E-04 | 0% |
| tyrosine (uirne) | 0.44 | 0.32 | 0.56 | 3.8E-13 | 0% |
| C10 | -0.23 | -0.35 | -0.11 | 2.6E-04 | 26% |
| C12 | -0.29 | -0.42 | -0.17 | 1.7E-06 | 18% |
| C14:1 | -0.34 | -0.46 | -0.21 | 7.0E-08 | 12% |
| C14:1-OH | -0.23 | -0.35 | -0.11 | 2.1E-04 | 15% |
| C14:2 | -0.24 | -0.36 | -0.12 | 9.2E-05 | 13% |
| C16:1 | -0.26 | -0.38 | -0.14 | 2.4E-05 | 0% |
| Lys | -0.24 | -0.36 | -0.12 | 9.4E-05 | 53% |
| Orn | -0.35 | -0.47 | -0.23 | 2.1E-08 | 20% |
| Ser | -0.26 | -0.39 | -0.14 | 2.2E-05 | 8% |
| Putrescine | -0.27 | -0.38 | -0.15 | 6.4E-06 | 39% |
| Serotonin | 0.32 | 0.20 | 0.44 | 1.6E-07 | 54% |
| SM C16:1 | -0.35 | -0.46 | -0.24 | 3.2E-10 | 0% |
| SM C18:0 | -0.22 | -0.33 | -0.11 | 9.6E-05 | 0% |
| SM C18:1 | -0.36 | -0.46 | -0.25 | 1.4E-10 | 0% |
| H1 | 0.23 | 0.11 | 0.35 | 2.4E-04 | 7% |

Metabolites found higher in male children are shown as positive and metabolites found higher in female children are shown as negative

## Supplementary Table 14 Modeled results with Box-Cox transformation and QRILC imputation - metabolites associated with BMI z-score

| metabolite | effect size (SD/ unit z-score) | lower CI | upper CI | p-value | $I^2$ |
|---|---|---|---|---|---|
| valine (urine) | 0.10 | 0.05 | 0.15 | 2.0E-04 | 0% |
| 4-deoxyerythronic acid (urine) | 0.21 | 0.16 | 0.26 | 5.7E-16 | 30% |
| *p*-cresol sulfate (urine) | -0.11 | -0.16 | -0.06 | 3.9E-05 | 57% |
| pantothenate (urine) | -0.12 | -0.17 | -0.07 | 2.2E-06 | 11% |
| C0 | 0.19 | 0.14 | 0.24 | 3.2E-13 | 0% |
| C18 | -0.13 | -0.18 | -0.08 | 8.1E-07 | 21% |
| C3 | 0.15 | 0.10 | 0.20 | 7.4E-10 | 0% |
| C5 | 0.13 | 0.08 | 0.19 | 4.0E-07 | 0% |
| Asp | 0.10 | 0.05 | 0.15 | 1.2E-04 | 13% |
| Glu | 0.22 | 0.17 | 0.27 | 3.7E-17 | 0% |
| Ile | 0.11 | 0.05 | 0.16 | 7.5E-05 | 0% |
| Leu | 0.12 | 0.07 | 0.17 | 4.9E-06 | 0% |
| Lys | 0.10 | 0.05 | 0.15 | 1.3E-04 | 0% |
| Phe | 0.13 | 0.07 | 0.18 | 1.4E-06 | 12% |
| Pro | 0.10 | 0.05 | 0.15 | 1.3E-04 | 0% |
| Tyr | 0.10 | 0.05 | 0.15 | 2.7E-04 | 0% |
| Val | 0.13 | 0.08 | 0.19 | 4.1E-07 | 0% |
| ADMA | 0.10 | 0.04 | 0.15 | 2.5E-04 | 0% |
| alpha-AAA | 0.10 | 0.05 | 0.15 | 8.7E-05 | 0% |
| Kynurenine | 0.10 | 0.05 | 0.15 | 1.1E-04 | 37% |
| lysoPC a C16:1 | 0.14 | 0.09 | 0.19 | 9.5E-08 | 0% |
| lysoPC a C18:1 | -0.09 | -0.14 | -0.04 | 1.9E-04 | 0% |
| lysoPC a C18:2 | -0.12 | -0.17 | -0.07 | 4.9E-06 | 0% |
| PC aa C32:1 | 0.11 | 0.06 | 0.16 | 1.7E-05 | 0% |
| PC aa C32:3 | 0.10 | 0.05 | 0.15 | 5.2E-05 | 0% |
| PC aa C34:4 | 0.13 | 0.08 | 0.19 | 2.4E-07 | 0% |
| PC aa C36:5 | 0.10 | 0.05 | 0.15 | 1.4E-04 | 0% |
| PC aa C36:6 | 0.10 | 0.04 | 0.15 | 2.6E-04 | 0% |
| PC aa C38:1 | -0.10 | -0.15 | -0.05 | 1.4E-04 | 32% |
| PC aa C38:3 | 0.20 | 0.15 | 0.25 | 5.7E-16 | 0% |
| PC aa C38:4 | 0.13 | 0.08 | 0.19 | 1.5E-07 | 0% |
| PC aa C40:6 | 0.10 | 0.05 | 0.15 | 1.2E-04 | 0% |
| PC ae C34:0 | -0.09 | -0.14 | -0.04 | 1.9E-04 | 0% |
| PC ae C34:1 | -0.09 | -0.14 | -0.04 | 2.6E-04 | 0% |
| PC ae C36:0 | -0.10 | -0.15 | -0.05 | 2.3E-05 | 0% |
| PC ae C36:2 | -0.12 | -0.17 | -0.07 | 2.0E-06 | 0% |
| PC ae C38:2 | -0.10 | -0.15 | -0.05 | 5.2E-05 | 0% |
| PC ae C40:4 | -0.11 | -0.16 | -0.06 | 2.1E-05 | 21% |
| PC ae C40:5 | -0.10 | -0.15 | -0.05 | 1.0E-04 | 12% |
| PC ae C40:6 | -0.10 | -0.15 | -0.05 | 1.5E-04 | 0% |
| PC ae C42:3 | -0.11 | -0.16 | -0.06 | 1.6E-05 | 0% |
| PC ae C42:4 | -0.14 | -0.19 | -0.09 | 1.6E-07 | 0% |
| PC ae C44:4 | -0.11 | -0.16 | -0.05 | 6.7E-05 | 23% |
| SM C16:0 | -0.10 | -0.14 | -0.05 | 7.3E-05 | 17% |
| SM C16:1 | 0.16 | 0.12 | 0.21 | 1.3E-11 | 0% |
| SM C18:1 | 0.15 | 0.11 | 0.20 | 8.9E-11 | 0% |

## Supplementary Table 15 Modeled results with Box-Cox transformation and QRILC imputation - metabolites associated with dietary intake

| metabolite-diet pair | effect size (SD/ times per week) | lower CI | upper CI | p-value | $I^2$ |
|---|---|---|---|---|---|
| creatine (urine) with meat | 0.027 | 0.013 | 0.040 | 1.3E-04 | 0% |
| pantothenate (urine) with dairy | 0.009 | 0.004 | 0.015 | 7.5E-04 | 37% |
| hippurate (urine) with vegetables | 0.021 | 0.011 | 0.031 | 2.6E-05 | 0% |
| leucine (urine) with fruits | -0.014 | -0.022 | -0.006 | 6.0E-04 | 0% |
| threonine/ lactate (urine) with fruits | -0.013 | -0.021 | -0.005 | 9.6E-04 | 19% |
| alanine (urine) with fruits | -0.014 | -0.022 | -0.006 | 7.7E-04 | 29% |
| succinate (urine) with fruits | 0.015 | 0.007 | 0.023 | 1.7E-04 | 30% |
| glutamine (urine) with fruits | -0.020 | -0.028 | -0.013 | 3.4E-07 | 0% |
| *scyllo*-inositol (urine) with fruits | 0.018 | 0.011 | 0.025 | 3.0E-07 | 58% |
| hippurate (urine) with fruits | 0.026 | 0.018 | 0.034 | 4.4E-11 | 50% |
| 3-aminoisobutyrate (urine) with fruits | 0.015 | 0.007 | 0.023 | 1.9E-04 | 24% |
| proline betaine (urine) with fruits | 0.023 | 0.015 | 0.031 | 1.5E-08 | 19% |
| *N*-methylnicotinic acid (urine) with fruits | 0.018 | 0.010 | 0.026 | 1.6E-05 | 60% |
| 3-hydroxybutyrate/ 3-aminoisobutyrate (urine) with beverages | -0.034 | -0.053 | -0.016 | 3.2E-04 | 0% |
| PC ae C36:3 with meat | 0.024 | 0.011 | 0.037 | 2.3E-04 | 0% |
| PC ae C36:4 with meat | 0.031 | 0.018 | 0.044 | 3.5E-06 | 0% |
| PC ae C36:5 with meat | 0.026 | 0.013 | 0.040 | 1.1E-04 | 0% |
| PC ae C38:5 with meat | 0.027 | 0.014 | 0.040 | 5.7E-05 | 20% |
| PC aa C36:0 with fish | 0.091 | 0.064 | 0.119 | 9.0E-11 | 56% |
| PC aa C36:5 with fish | 0.063 | 0.035 | 0.091 | 1.3E-05 | 43% |
| PC aa C36:6 with fish | 0.087 | 0.059 | 0.114 | 7.9E-10 | 0% |
| PC aa C38:0 with fish | 0.108 | 0.081 | 0.135 | 9.1E-15 | 74% |
| PC aa C38:6 with fish | 0.113 | 0.085 | 0.140 | 1.2E-15 | 57% |
| PC aa C40:1 with fish | 0.055 | 0.027 | 0.082 | 1.1E-04 | 0% |
| PC aa C40:4 with fish | -0.057 | -0.084 | -0.030 | 3.5E-05 | 19% |
| PC aa C40:6 with fish | 0.100 | 0.072 | 0.128 | 1.5E-12 | 48% |
| PC aa C42:0 with fish | 0.052 | 0.024 | 0.080 | 2.4E-04 | 0% |
| PC aa C42:2 with fish | 0.057 | 0.029 | 0.084 | 5.3E-05 | 3% |
| PC ae C32:2 with fish | 0.047 | 0.022 | 0.072 | 2.3E-04 | 36% |
| PC ae C38:0 with fish | 0.086 | 0.058 | 0.113 | 8.7E-10 | 37% |
| PC ae C38:6 with fish | 0.074 | 0.046 | 0.102 | 1.9E-07 | 56% |
| PC ae C40:6 with fish | 0.087 | 0.059 | 0.115 | 9.0E-10 | 31% |
| Gly with dairy | -0.010 | -0.016 | -0.005 | 2.8E-04 | 31% |
| PC aa C28:1 with dairy | 0.015 | 0.010 | 0.020 | 3.5E-08 | 59% |
| PC aa C30:0 with dairy | 0.012 | 0.007 | 0.017 | 1.6E-05 | 69% |
| PC aa C38:0 with dairy | -0.013 | -0.018 | -0.008 | 2.1E-06 | 0% |
| PC ae C30:0 with dairy | 0.015 | 0.009 | 0.020 | 3.0E-08 | 73% |
| PC ae C38:6 with dairy | -0.010 | -0.016 | -0.005 | 2.2E-04 | 0% |
| SM (OH) C14:1 with dairy | 0.013 | 0.007 | 0.018 | 3.4E-06 | 71% |
| PC ae C30:0 with potatoes | -0.042 | -0.064 | -0.020 | 1.7E-04 | 0% |
| PC ae C34:0 with potatoes | -0.048 | -0.070 | -0.026 | 1.7E-05 | 29% |
| SM (OH) C14:1 with potatoes | -0.046 | -0.067 | -0.024 | 4.0E-05 | 50% |
| Ac-Orn with fruits | 0.016 | 0.008 | 0.023 | 7.5E-05 | 0% |
| PC aa C38:0 with sweets | -0.022 | -0.032 | -0.012 | 1.3E-05 | 0% |
| PC aa C38:6 with sweets | -0.022 | -0.032 | -0.011 | 3.1E-05 | 0% |
| PC ae C38:5 with sweets | -0.021 | -0.031 | -0.011 | 2.3E-05 | 23% |
| PC ae C38:6 with sweets | -0.021 | -0.031 | -0.011 | 5.2E-05 | 0% |
| PC ae C40:6 with sweets | -0.023 | -0.033 | -0.013 | 8.4E-06 | 0% |
| lysoPC a C17:0 with bakery products | -0.026 | -0.039 | -0.013 | 6.4E-05 | 49% |
| PC aa C36:6 with bakery products | -0.027 | -0.040 | -0.014 | 4.2E-05 | 0% |
| PC aa C38:0 with bakery products | -0.026 | -0.039 | -0.014 | 5.0E-05 | 51% |
| PC aa C38:6 with bakery products | -0.027 | -0.040 | -0.014 | 4.3E-05 | 54% |
| PC aa C40:6 with bakery products | -0.027 | -0.040 | -0.014 | 4.3E-05 | 41% |
| PC ae C38:0 with bakery products | -0.030 | -0.042 | -0.017 | 4.5E-06 | 18% |
| PC ae C38:6 with bakery products | -0.025 | -0.037 | -0.012 | 1.9E-04 | 11% |
| PC ae C40:2 with bakery products | -0.027 | -0.039 | -0.014 | 4.5E-05 | 53% |
| PC ae C40:6 with bakery products | -0.025 | -0.038 | -0.013 | 9.5E-05 | 35% |
| SM (OH) C14:1 with bakery products | -0.027 | -0.039 | -0.014 | 3.6E-05 | 14% |
| SM (OH) C16:1 with bakery products | -0.030 | -0.042 | -0.018 | 1.6E-06 | 32% |
| C5:1 with beverages | -0.033 | -0.050 | -0.015 | 2.1E-04 | 1% |
| C6:1 with beverages | -0.031 | -0.047 | -0.015 | 1.6E-04 | 20% |