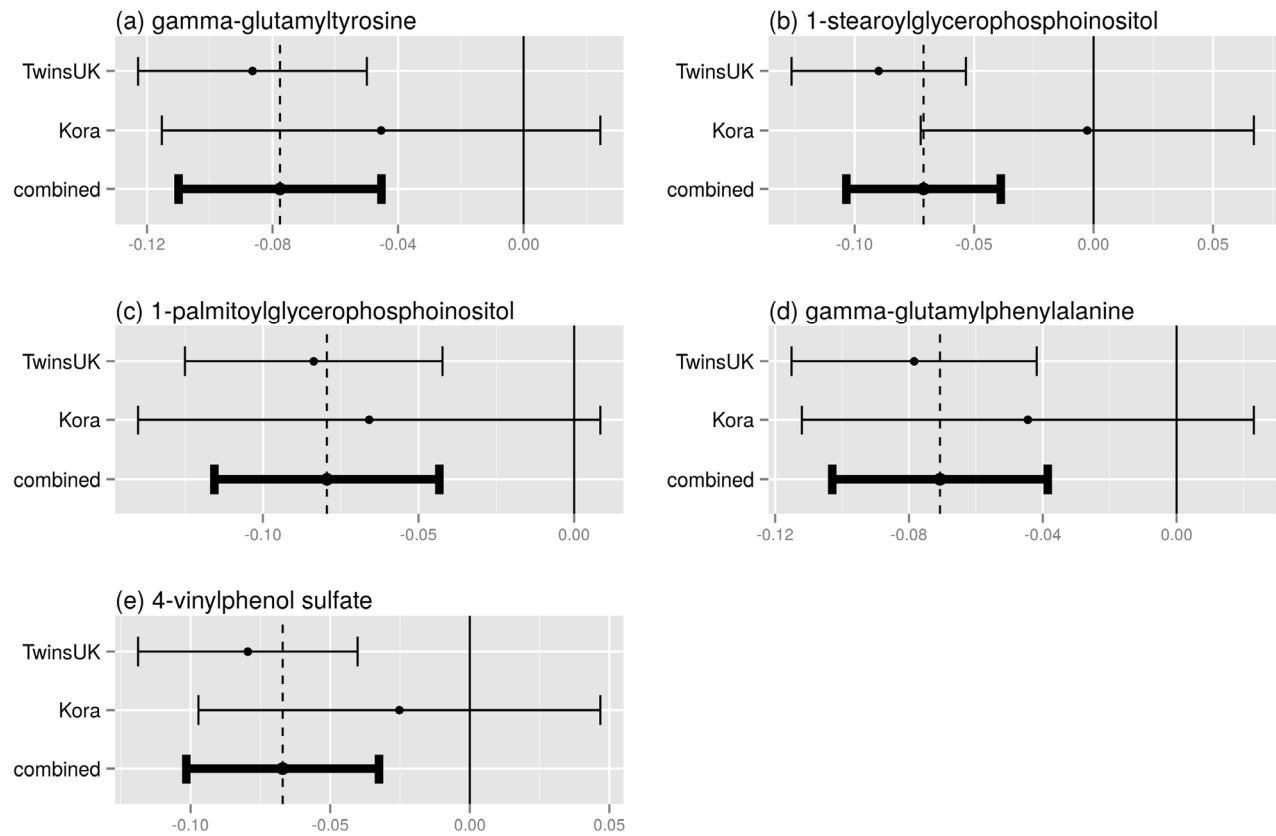


SUPPLEMENTAL DATA



Supplemental Figure 1. Forest plots of significant metabolites. The forest plots show effects and confidence intervals for all significant metabolites in the discovery cohort (TwinsUK), the replication cohort (Kora) and the combined meta-analysis. The dashed lines indicate the combined effect after meta-analysis.

Supplemental Table 1. Associations of blood metabolite levels with LTL. The table contains the complete list of all analyzed metabolites and their association with LTL. (indicates FWER<0.05, * indicates FDR <0.05)**

| metabolite | pathway | beta [95%CI] | p |
|--|------------------------|---------------------|-------------------------|
| 1-stearoylglycerophosphoinositol | Lipid | -0.09 [-0.13:-0.05] | 1.36×10 ^{-6**} |
| gamma-glutamyltyrosine | Peptide | -0.09 [-0.12:-0.05] | 3.41×10 ^{-6**} |
| gamma-glutamylphenylalanine | Peptide | -0.08 [-0.12:-0.04] | 2.72×10 ^{-5**} |
| 1-palmitoylglycerophosphoinositol | Lipid | -0.08 [-0.13:-0.04] | 7.36×10 ^{-5**} |
| 4-vinylphenol sulfate | Xenobiotics | -0.08 [-0.12:-0.04] | 7.41×10 ^{-5**} |
| 1-arachidonoylglycerophosphoethanolamine | Lipid | -0.07 [-0.11:-0.03] | 2.42×10 ^{-4*} |
| 1-arachidonoylglycerophosphoinositol | Lipid | -0.07 [-0.11:-0.03] | 2.76×10 ^{-4*} |
| 1-oleoylglycerophosphoethanolamine | Lipid | -0.07 [-0.10:-0.03] | 7.60×10 ^{-4*} |
| uridine | Nucleotide | 0.06 [0.03:0.10] | 1.07×10 ^{-3*} |
| caprylate (8:0) | Lipid | -0.06 [-0.10:-0.02] | 1.42×10 ^{-3*} |
| erythritol | Xenobiotics | -0.06 [-0.09:-0.02] | 1.54×10 ^{-3*} |
| arabinose | Carbohydrate | -0.07 [-0.11:-0.02] | 1.75×10 ^{-3*} |
| ornithine | Amino acid | -0.06 [-0.10:-0.02] | 2.14×10 ^{-3*} |
| heptanoate (7:0) | Lipid | -0.06 [-0.09:-0.02] | 3.25×10 ⁻³ |
| pyroglutamine | Amino acid | -0.05 [-0.09:-0.02] | 3.54×10 ⁻³ |
| tyrosine | Amino acid | -0.05 [-0.09:-0.02] | 5.27×10 ⁻³ |
| laurylcarnitine | Lipid | -0.07 [-0.11:-0.02] | 6.70×10 ⁻³ |
| proline | Amino acid | -0.05 [-0.09:-0.01] | 7.56×10 ⁻³ |
| malate | Energy | -0.05 [-0.09:-0.01] | 7.66×10 ⁻³ |
| caproate (6:0) | Lipid | -0.05 [-0.09:-0.01] | 7.66×10 ⁻³ |
| kynurenine | Amino acid | -0.05 [-0.08:-0.01] | 1.04×10 ⁻² |
| pseudouridine | Nucleotide | -0.05 [-0.08:-0.01] | 1.30×10 ⁻² |
| 1-palmitoylglycerophosphoethanolamine | Lipid | -0.05 [-0.08:-0.01] | 1.31×10 ⁻² |
| arachidonate (20:4n6) | Lipid | -0.05 [-0.09:-0.01] | 1.33×10 ⁻² |
| 3-dehydrocarnitine | Lipid | -0.05 [-0.08:-0.01] | 1.41×10 ⁻² |
| C-glycosyltryptophan | Amino acid | -0.04 [-0.08:-0.01] | 1.41×10 ⁻² |
| 1,3,7-trimethylurate | Xenobiotics | -0.06 [-0.11:-0.01] | 1.43×10 ⁻² |
| 4-methyl-2-oxopentanoate | Amino acid | 0.05 [0.01:0.08] | 1.56×10 ⁻² |
| bilirubin (E,E) | Cofactors and vitamins | 0.05 [0.01:0.08] | 1.58×10 ⁻² |
| p-acetamidophenylglucuronide | Xenobiotics | -0.09 [-0.17:-0.02] | 1.59×10 ⁻² |
| glycerol | Lipid | -0.05 [-0.08:-0.01] | 1.65×10 ⁻² |
| 1-eicosatrienoylglycerophosphocholine | Lipid | -0.05 [-0.08:-0.01] | 1.72×10 ⁻² |
| lactate | Carbohydrate | -0.05 [-0.08:-0.01] | 1.78×10 ⁻² |
| thromboxane B2 | Lipid | -0.04 [-0.08:-0.01] | 2.25×10 ⁻² |
| 1-palmitoylglycerol (1-monopalmitin) | Lipid | -0.04 [-0.08:-0.01] | 2.34×10 ⁻² |
| butyrylcarnitine | Lipid | -0.04 [-0.08:-0.01] | 2.37×10 ⁻² |
| 2-hydroxyglutarate | Lipid | -0.05 [-0.10:-0.01] | 2.38×10 ⁻² |
| homocitrulline | Amino acid | -0.06 [-0.12:-0.01] | 2.74×10 ⁻² |
| phenylalanine | Amino acid | -0.04 [-0.08:-0.00] | 2.74×10 ⁻² |
| alpha-hydroxyisovalerate | Amino acid | -0.04 [-0.08:-0.00] | 3.01×10 ⁻² |
| CMPF | Lipid | 0.04 [0.00:0.07] | 3.16×10 ⁻² |

| | | | |
|---|------------------------|---------------------|-----------------------|
| biliverdin | Cofactors and vitamins | 0.04 [0.00:0.08] | 3.47×10 ⁻² |
| cholesterol | Lipid | -0.04 [-0.07:-0.00] | 3.64×10 ⁻² |
| oleoylcarnitine | Lipid | 0.04 [0.00:0.08] | 3.83×10 ⁻² |
| pelargonate (9:0) | Lipid | -0.04 [-0.07:-0.00] | 4.00×10 ⁻² |
| paraxanthine | Xenobiotics | -0.04 [-0.08:-0.00] | 4.15×10 ⁻² |
| 3-(cystein-S-yl)acetaminophen | Xenobiotics | -0.09 [-0.18:-0.00] | 4.15×10 ⁻² |
| urate | Nucleotide | -0.04 [-0.07:-0.00] | 4.18×10 ⁻² |
| carnitine | Lipid | -0.04 [-0.08:-0.00] | 4.35×10 ⁻² |
| 1-linoleoylglycerophosphoethanolamine | Lipid | -0.04 [-0.08:-0.00] | 4.44×10 ⁻² |
| 1-stearoylglycerophosphoethanolamine | Lipid | -0.04 [-0.08:-0.00] | 4.46×10 ⁻² |
| adrenate (22:4n6) | Lipid | -0.04 [-0.08:-0.00] | 4.49×10 ⁻² |
| gamma-glutamylvaline | Peptide | -0.04 [-0.07:-0.00] | 4.83×10 ⁻² |
| threonate | Cofactors and vitamins | 0.04 [0.00:0.08] | 4.96×10 ⁻² |
| tetradecanedioate | Lipid | -0.04 [-0.08:0.00] | 5.11×10 ⁻² |
| hyodeoxycholate | Lipid | -0.04 [-0.08:0.00] | 5.11×10 ⁻² |
| 2-hydroxystearate | Lipid | -0.04 [-0.07:0.00] | 5.18×10 ⁻² |
| ibuprofen | Xenobiotics | -0.07 [-0.13:0.00] | 5.21×10 ⁻² |
| 2-methoxyacetaminophen sulfate | Xenobiotics | -0.08 [-0.17:0.00] | 5.22×10 ⁻² |
| 2-hydroxypalmitate | Lipid | -0.04 [-0.07:0.00] | 5.24×10 ⁻² |
| hexadecanedioate | Lipid | -0.04 [-0.08:0.00] | 5.36×10 ⁻² |
| gamma-glutamylthreonine | Peptide | -0.06 [-0.11:0.00] | 5.55×10 ⁻² |
| alanine | Amino acid | -0.04 [-0.07:0.00] | 5.73×10 ⁻² |
| dihomo-linolenate (20:3n3 or n6) | Lipid | -0.04 [-0.07:0.00] | 5.88×10 ⁻² |
| undecanoate (11:0) | Lipid | -0.04 [-0.07:0.00] | 6.04×10 ⁻² |
| glutamate | Amino acid | -0.03 [-0.07:0.00] | 6.14×10 ⁻² |
| glycerate | Carbohydrate | 0.03 [-0.00:0.07] | 7.26×10 ⁻² |
| ADpSGEGDFXAEGGGVR | Peptide | 0.06 [-0.01:0.12] | 7.39×10 ⁻² |
| naproxen | Xenobiotics | -0.33 [-0.68:0.02] | 8.20×10 ⁻² |
| saccharin | Xenobiotics | -0.06 [-0.12:0.01] | 8.32×10 ⁻² |
| aspartylphenylalanine | Peptide | -0.05 [-0.12:0.01] | 8.33×10 ⁻² |
| beta-hydroxyisovalerate | Amino acid | -0.03 [-0.07:0.00] | 8.51×10 ⁻² |
| propionylcarnitine | Lipid | -0.03 [-0.07:0.00] | 8.61×10 ⁻² |
| 7-Hoca | Lipid | -0.03 [-0.07:0.00] | 8.69×10 ⁻² |
| cyclo(leu-pro) | Peptide | -0.04 [-0.09:0.01] | 8.73×10 ⁻² |
| estrone 3-sulfate | Lipid | -0.09 [-0.18:0.01] | 8.92×10 ⁻² |
| benzoate | Xenobiotics | -0.03 [-0.07:0.01] | 9.32×10 ⁻² |
| 1-methylxanthine | Xenobiotics | -0.04 [-0.08:0.01] | 9.34×10 ⁻² |
| N-acetylalanine | Amino acid | -0.03 [-0.07:0.01] | 9.61×10 ⁻² |
| pyridoxate | Cofactors and vitamins | 0.03 [-0.01:0.07] | 9.70×10 ⁻² |
| 4-acetamidobutanoate | Amino acid | -0.03 [-0.07:0.01] | 9.80×10 ⁻² |
| gamma-glutamylleucine | Peptide | -0.03 [-0.07:0.01] | 1.01×10 ⁻¹ |
| 4-androsten-3beta,17beta-diol disulfate 1 | Lipid | -0.03 [-0.07:0.01] | 1.07×10 ⁻¹ |
| 1-arachidonoylglycerophosphocholine | Lipid | -0.03 [-0.07:0.01] | 1.07×10 ⁻¹ |
| 1-palmitoylplasménylethanolamine | Lipid | -0.03 [-0.08:0.01] | 1.07×10 ⁻¹ |
| 2-hydroxyisobutyrate | Amino acid | 0.03 [-0.01:0.07] | 1.11×10 ⁻¹ |

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|--------------------------------------|------------------------|--------------------|-----------------------|
| cafféine | Xenobiotics | -0.03 [-0.07:0.01] | 1.15×10 ⁻¹ |
| 3-methyl-2-oxovalerate | Amino acid | 0.03 [-0.01:0.07] | 1.20×10 ⁻¹ |
| 4-acetamidophenol | Xenobiotics | -0.08 [-0.18:0.02] | 1.23×10 ⁻¹ |
| N2,N2-dimethylguanosine | Nucleotide | -0.03 [-0.07:0.01] | 1.34×10 ⁻¹ |
| cholate | Lipid | 0.03 [-0.01:0.08] | 1.36×10 ⁻¹ |
| succinylcarnitine | Energy | -0.03 [-0.07:0.01] | 1.38×10 ⁻¹ |
| stachydrine | Xenobiotics | 0.03 [-0.01:0.07] | 1.40×10 ⁻¹ |
| citrate | Energy | 0.03 [-0.01:0.06] | 1.42×10 ⁻¹ |
| 1-palmitoleoylglycerophosphocholine | Lipid | -0.03 [-0.07:0.01] | 1.44×10 ⁻¹ |
| gamma-glutamylisoleucine | Peptide | -0.03 [-0.07:0.01] | 1.47×10 ⁻¹ |
| phenyllactate | Amino acid | -0.03 [-0.07:0.01] | 1.51×10 ⁻¹ |
| hydroxyisovaleroyl carnitine | Amino acid | -0.03 [-0.08:0.01] | 1.54×10 ⁻¹ |
| isoleucine | Amino acid | -0.03 [-0.06:0.01] | 1.55×10 ⁻¹ |
| palmitate (16:0) | Lipid | -0.03 [-0.07:0.01] | 1.58×10 ⁻¹ |
| 1,7-dimethylurate | Xenobiotics | -0.03 [-0.07:0.01] | 1.59×10 ⁻¹ |
| creatinine | Amino acid | -0.03 [-0.06:0.01] | 1.61×10 ⁻¹ |
| 3-(3-hydroxyphenyl)propionate | Amino acid | 0.07 [-0.03:0.16] | 1.64×10 ⁻¹ |
| 4-hydroxyhippurate | Xenobiotics | -0.03 [-0.08:0.01] | 1.65×10 ⁻¹ |
| N-acetylmornithine | Amino acid | -0.03 [-0.07:0.01] | 1.82×10 ⁻¹ |
| N-(2-furoyl)glycine | Xenobiotics | -0.10 [-0.25:0.05] | 1.87×10 ⁻¹ |
| palmitoylcarnitine | Lipid | 0.02 [-0.01:0.06] | 2.02×10 ⁻¹ |
| 1-heptadecanoylglycerophosphocholine | Lipid | 0.03 [-0.01:0.06] | 2.05×10 ⁻¹ |
| histidine | Amino acid | 0.02 [-0.01:0.06] | 2.08×10 ⁻¹ |
| 4-ethylphenylsulfate | Xenobiotics | -0.03 [-0.07:0.02] | 2.09×10 ⁻¹ |
| 3-methyl-2-oxobutyrate | Amino acid | 0.02 [-0.01:0.06] | 2.09×10 ⁻¹ |
| phenol sulfate | Amino acid | -0.02 [-0.06:0.01] | 2.11×10 ⁻¹ |
| 1,5-anhydroglucitol (1,5-AG) | Carbohydrate | -0.02 [-0.06:0.01] | 2.12×10 ⁻¹ |
| alpha-tocopherol | Cofactors and vitamins | 0.02 [-0.01:0.06] | 2.20×10 ⁻¹ |
| 2-hydroxyacetaminophen sulfate | Xenobiotics | -0.04 [-0.12:0.03] | 2.23×10 ⁻¹ |
| mannose | Carbohydrate | -0.02 [-0.06:0.01] | 2.27×10 ⁻¹ |
| glycochenodeoxycholate | Lipid | -0.02 [-0.06:0.02] | 2.36×10 ⁻¹ |
| piperine | Xenobiotics | 0.02 [-0.02:0.06] | 2.38×10 ⁻¹ |
| deoxycholate | Lipid | -0.03 [-0.08:0.02] | 2.39×10 ⁻¹ |
| nonadecanoate (19:0) | Lipid | 0.02 [-0.01:0.06] | 2.41×10 ⁻¹ |
| hippurate | Xenobiotics | 0.02 [-0.02:0.06] | 2.42×10 ⁻¹ |
| 3-indoxyl sulfate | Amino acid | -0.02 [-0.06:0.02] | 2.52×10 ⁻¹ |
| bilirubin (Z,Z) | Cofactors and vitamins | 0.02 [-0.02:0.06] | 2.55×10 ⁻¹ |
| myristate (14:0) | Lipid | -0.02 [-0.06:0.02] | 2.56×10 ⁻¹ |
| hexanoylcarnitine | Lipid | -0.02 [-0.06:0.02] | 2.61×10 ⁻¹ |
| 2-tetradecenoyl carnitine | Lipid | -0.02 [-0.06:0.02] | 2.63×10 ⁻¹ |
| myo-inositol | Lipid | -0.02 [-0.06:0.02] | 2.70×10 ⁻¹ |
| palmitoyl sphingomyelin | Lipid | -0.02 [-0.06:0.02] | 2.70×10 ⁻¹ |
| palmitoleate (16:1n7) | Lipid | -0.02 [-0.06:0.02] | 2.74×10 ⁻¹ |
| ursodeoxycholate | Lipid | -0.02 [-0.07:0.02] | 2.77×10 ⁻¹ |
| homostachydrine | Xenobiotics | -0.04 [-0.11:0.03] | 2.78×10 ⁻¹ |

| | | | |
|--|------------------------|--------------------|-----------------------|
| lathosterol | Lipid | -0.02 [-0.06:0.02] | 2.84×10 ⁻¹ |
| laurate (12:0) | Lipid | -0.02 [-0.06:0.02] | 2.86×10 ⁻¹ |
| 3-phenylpropionate (hydrocinnamate) | Amino acid | 0.02 [-0.02:0.06] | 2.86×10 ⁻¹ |
| glutaroyl carnitine | Amino acid | -0.02 [-0.06:0.02] | 2.88×10 ⁻¹ |
| DHA (22:6n3) | Lipid | 0.02 [-0.02:0.06] | 2.92×10 ⁻¹ |
| bradykinin, des-arg(9) | Peptide | 0.03 [-0.02:0.08] | 3.01×10 ⁻¹ |
| 7-methylxanthine | Xenobiotics | 0.02 [-0.02:0.07] | 3.05×10 ⁻¹ |
| erythrose | Carbohydrate | 0.02 [-0.02:0.06] | 3.07×10 ⁻¹ |
| epiandrosterone sulfate | Lipid | -0.02 [-0.05:0.02] | 3.13×10 ⁻¹ |
| 1-stearoylglycerol (1-monostearin) | Lipid | -0.02 [-0.06:0.02] | 3.13×10 ⁻¹ |
| 10-heptadecenoate (17:1n7) | Lipid | -0.02 [-0.06:0.02] | 3.23×10 ⁻¹ |
| glucose | Carbohydrate | -0.02 [-0.06:0.02] | 3.37×10 ⁻¹ |
| myristoleate (14:1n5) | Lipid | -0.02 [-0.06:0.02] | 3.38×10 ⁻¹ |
| 10-undecenoate (11:1n1) | Lipid | 0.02 [-0.02:0.06] | 3.41×10 ⁻¹ |
| threonine | Amino acid | -0.02 [-0.06:0.02] | 3.45×10 ⁻¹ |
| taurochenodeoxycholate | Lipid | -0.02 [-0.06:0.02] | 3.45×10 ⁻¹ |
| salicylicuric glucuronide | Xenobiotics | -0.06 [-0.19:0.07] | 3.50×10 ⁻¹ |
| 5alpha-androstan-3beta,17beta-diol disulfate | Lipid | -0.02 [-0.06:0.02] | 3.54×10 ⁻¹ |
| 1-methylurate | Xenobiotics | -0.02 [-0.06:0.02] | 3.56×10 ⁻¹ |
| dodecanedioate | Lipid | -0.02 [-0.06:0.02] | 3.56×10 ⁻¹ |
| GPC | Lipid | -0.02 [-0.06:0.02] | 3.57×10 ⁻¹ |
| tryptophan | Amino acid | 0.02 [-0.02:0.06] | 3.62×10 ⁻¹ |
| 1-oleoylglycerol (1-monoolein) | Lipid | -0.02 [-0.07:0.02] | 3.64×10 ⁻¹ |
| catechol sulfate | Xenobiotics | -0.02 [-0.06:0.02] | 3.64×10 ⁻¹ |
| mannitol | Carbohydrate | -0.02 [-0.06:0.02] | 3.71×10 ⁻¹ |
| pantothenate | Cofactors and vitamins | 0.02 [-0.02:0.06] | 3.74×10 ⁻¹ |
| gamma-tocopherol | Cofactors and vitamins | -0.02 [-0.06:0.02] | 3.76×10 ⁻¹ |
| asparagine | Amino acid | 0.02 [-0.02:0.05] | 3.79×10 ⁻¹ |
| 1-stearoylglycerophosphocholine | Lipid | 0.02 [-0.02:0.05] | 3.83×10 ⁻¹ |
| lysine | Amino acid | -0.02 [-0.05:0.02] | 3.83×10 ⁻¹ |
| stearoylcarnitine | Lipid | 0.02 [-0.02:0.05] | 3.89×10 ⁻¹ |
| 2-stearoylglycerophosphocholine | Lipid | 0.02 [-0.02:0.05] | 3.93×10 ⁻¹ |
| 2-methylbutyrylcarnitine | Amino acid | -0.02 [-0.05:0.02] | 4.03×10 ⁻¹ |
| 1,6-anhydroglucose | Carbohydrate | -0.02 [-0.07:0.03] | 4.07×10 ⁻¹ |
| glycocholate | Lipid | 0.02 [-0.02:0.06] | 4.08×10 ⁻¹ |
| leucine | Amino acid | -0.02 [-0.05:0.02] | 4.10×10 ⁻¹ |
| 15-methylpalmitate (isobar with 2-methylpalmitate) | Lipid | -0.02 [-0.06:0.03] | 4.14×10 ⁻¹ |
| acetylphosphate | Energy | -0.01 [-0.05:0.02] | 4.31×10 ⁻¹ |
| 5alpha-pregnan-3beta,20alpha-diol disulfate | Lipid | 0.02 [-0.03:0.06] | 4.42×10 ⁻¹ |
| cysteine | Amino acid | -0.01 [-0.05:0.02] | 4.43×10 ⁻¹ |
| phenylacetate | Amino acid | 0.02 [-0.03:0.06] | 4.54×10 ⁻¹ |
| n-Butyl Oleate | Lipid | 0.02 [-0.03:0.07] | 4.56×10 ⁻¹ |
| cis-4-decenoyl carnitine | Lipid | -0.02 [-0.06:0.03] | 4.58×10 ⁻¹ |
| creatine | Amino acid | 0.01 [-0.02:0.05] | 4.67×10 ⁻¹ |
| 3-(4-hydroxyphenyl)lactate | Amino acid | -0.01 [-0.05:0.02] | 4.74×10 ⁻¹ |

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|---|--------------|--------------------|-----------------------|
| 7-methylguanine | Nucleotide | -0.02 [-0.06:0.03] | 4.88×10 ⁻¹ |
| citrulline | Amino acid | -0.01 [-0.05:0.02] | 4.93×10 ⁻¹ |
| DHEA-S | Lipid | -0.01 [-0.04:0.02] | 5.03×10 ⁻¹ |
| pentadecanoate (15:0) | Lipid | -0.01 [-0.05:0.03] | 5.10×10 ⁻¹ |
| 5-dodecenoate (12:1n7) | Lipid | -0.01 [-0.05:0.03] | 5.13×10 ⁻¹ |
| 4-androsten-3beta,17beta-diol disulfate 2 | Lipid | -0.01 [-0.05:0.03] | 5.15×10 ⁻¹ |
| arginine | Amino acid | 0.01 [-0.03:0.05] | 5.19×10 ⁻¹ |
| linoleate (18:2n6) | Lipid | -0.01 [-0.05:0.03] | 5.27×10 ⁻¹ |
| octanoylcarnitine | Lipid | -0.01 [-0.05:0.03] | 5.32×10 ⁻¹ |
| atenolol | Xenobiotics | -0.06 [-0.25:0.13] | 5.39×10 ⁻¹ |
| phenylalanylphenylalanine | Peptide | 0.02 [-0.04:0.08] | 5.40×10 ⁻¹ |
| tryptophan betaine | Amino acid | 0.01 [-0.03:0.05] | 5.42×10 ⁻¹ |
| androsterone sulfate | Lipid | -0.01 [-0.05:0.02] | 5.44×10 ⁻¹ |
| N-acetylthreonine | Amino acid | -0.01 [-0.05:0.03] | 5.46×10 ⁻¹ |
| 2-hydroxyhippurate (salicylurate) | Xenobiotics | 0.02 [-0.04:0.08] | 5.65×10 ⁻¹ |
| glycerol 2-phosphate | Xenobiotics | 0.01 [-0.03:0.05] | 5.90×10 ⁻¹ |
| dihomo-linoleate (20:2n6) | Lipid | -0.01 [-0.05:0.03] | 5.94×10 ⁻¹ |
| valine | Amino acid | -0.01 [-0.05:0.03] | 5.94×10 ⁻¹ |
| carbamazepine | Xenobiotics | 0.12 [-0.31:0.55] | 6.01×10 ⁻¹ |
| 3-hydroxybutyrate (BHBA) | Lipid | 0.01 [-0.03:0.05] | 6.05×10 ⁻¹ |
| N1-methyladenosine | Nucleotide | -0.01 [-0.05:0.03] | 6.16×10 ⁻¹ |
| betaine | Amino acid | 0.01 [-0.03:0.05] | 6.21×10 ⁻¹ |
| decanoylcarnitine | Lipid | 0.01 [-0.03:0.05] | 6.21×10 ⁻¹ |
| N-acetylglycine | Amino acid | 0.01 [-0.03:0.05] | 6.28×10 ⁻¹ |
| isovalerate | Lipid | -0.01 [-0.05:0.03] | 6.34×10 ⁻¹ |
| allantoin | Nucleotide | -0.01 [-0.05:0.03] | 6.40×10 ⁻¹ |
| chiro-inositol | Lipid | 0.02 [-0.05:0.08] | 6.42×10 ⁻¹ |
| salicylate | Xenobiotics | -0.01 [-0.08:0.05] | 6.47×10 ⁻¹ |
| glycine | Amino acid | 0.01 [-0.03:0.05] | 6.50×10 ⁻¹ |
| serine | Amino acid | 0.01 [-0.03:0.05] | 6.56×10 ⁻¹ |
| cotinine | Xenobiotics | 0.02 [-0.08:0.12] | 6.65×10 ⁻¹ |
| dimethylarginine (SDMA + ADMA) | Amino acid | 0.01 [-0.03:0.05] | 6.78×10 ⁻¹ |
| hypoxanthine | Nucleotide | -0.01 [-0.05:0.03] | 6.89×10 ⁻¹ |
| theobromine | Xenobiotics | -0.01 [-0.05:0.03] | 6.90×10 ⁻¹ |
| erythronate | Carbohydrate | 0.01 [-0.03:0.05] | 6.90×10 ⁻¹ |
| taurocholate | Lipid | 0.01 [-0.04:0.06] | 6.92×10 ⁻¹ |
| alpha-ketoglutarate | Energy | 0.01 [-0.03:0.05] | 7.12×10 ⁻¹ |
| stearidonate (18:4n3) | Lipid | -0.01 [-0.04:0.03] | 7.13×10 ⁻¹ |
| 2-palmitoylglycerophosphocholine | Lipid | -0.01 [-0.04:0.03] | 7.32×10 ⁻¹ |
| eicosenoate (20:1n9 or 11) | Lipid | 0.01 [-0.03:0.04] | 7.44×10 ⁻¹ |
| pyruvate | Carbohydrate | 0.01 [-0.03:0.04] | 7.54×10 ⁻¹ |
| valerate | Lipid | -0.01 [-0.06:0.04] | 7.55×10 ⁻¹ |
| fructose | Carbohydrate | 0.01 [-0.03:0.04] | 7.57×10 ⁻¹ |
| EPA | Lipid | 0.01 [-0.03:0.04] | 7.58×10 ⁻¹ |
| stearate (18:0) | Lipid | -0.01 [-0.04:0.03] | 7.61×10 ⁻¹ |

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| octadecanedioate | Lipid | 0.01 [-0.03:0.04] | 7.73×10 ⁻¹ |
| urea | Amino acid | -0.01 [-0.04:0.03] | 7.75×10 ⁻¹ |
| indoleacetate | Amino acid | 0.01 [-0.03:0.04] | 7.76×10 ⁻¹ |
| cortisone | Lipid | -0.01 [-0.04:0.03] | 7.76×10 ⁻¹ |
| levulinate (4-oxovalerate) | Amino acid | 0.01 [-0.03:0.04] | 7.80×10 ⁻¹ |
| oleate (18:1n9) | Lipid | -0.01 [-0.04:0.03] | 7.82×10 ⁻¹ |
| margarate (17:0) | Lipid | -0.01 [-0.04:0.03] | 7.83×10 ⁻¹ |
| 1-oleoylglycerophosphocholine | Lipid | 0.01 [-0.03:0.04] | 7.87×10 ⁻¹ |
| tauroolithocholate 3-sulfate | Lipid | -0.00 [-0.05:0.04] | 8.10×10 ⁻¹ |
| leucylleucine | Peptide | -0.01 [-0.06:0.05] | 8.21×10 ⁻¹ |
| ADSGEGDFXAEGGGVR | Peptide | 0.01 [-0.04:0.05] | 8.23×10 ⁻¹ |
| 3-methoxytyrosine | Amino acid | -0.00 [-0.05:0.04] | 8.26×10 ⁻¹ |
| 2-hydroxybutyrate (AHB) | Amino acid | 0.00 [-0.03:0.04] | 8.29×10 ⁻¹ |
| methionine | Amino acid | 0.00 [-0.03:0.04] | 8.31×10 ⁻¹ |
| pipecolate | Amino acid | -0.00 [-0.04:0.03] | 8.33×10 ⁻¹ |
| 2-oleoylglycerophosphocholine | Lipid | 0.00 [-0.03:0.04] | 8.36×10 ⁻¹ |
| 1-linoleoylglycerophosphocholine | Lipid | 0.00 [-0.03:0.04] | 8.40×10 ⁻¹ |
| scyllo-inositol | Lipid | 0.00 [-0.04:0.05] | 8.42×10 ⁻¹ |
| glutamine | Amino acid | -0.00 [-0.04:0.03] | 8.44×10 ⁻¹ |
| indolelactate | Amino acid | -0.00 [-0.04:0.03] | 8.47×10 ⁻¹ |
| heme | Cofactors and vitamins | 0.00 [-0.04:0.05] | 8.56×10 ⁻¹ |
| 2-aminobutyrate | Amino acid | 0.00 [-0.03:0.04] | 8.58×10 ⁻¹ |
| 10-nonadecenoate (19:1n9) | Lipid | -0.00 [-0.04:0.03] | 8.78×10 ⁻¹ |
| 1-myristoylglycerophosphocholine | Lipid | -0.00 [-0.04:0.03] | 8.80×10 ⁻¹ |
| thymol sulfate | Xenobiotics | -0.00 [-0.06:0.05] | 8.81×10 ⁻¹ |
| pro-hydroxy-pro | Peptide | 0.00 [-0.04:0.04] | 8.82×10 ⁻¹ |
| trans-4-hydroxyproline | Amino acid | 0.00 [-0.04:0.04] | 8.86×10 ⁻¹ |
| cortisol | Lipid | 0.00 [-0.04:0.04] | 8.87×10 ⁻¹ |
| 5-oxoproline | Amino acid | 0.00 [-0.04:0.04] | 8.91×10 ⁻¹ |
| threitol | Carbohydrate | -0.00 [-0.04:0.03] | 8.91×10 ⁻¹ |
| G3P | Lipid | 0.00 [-0.03:0.04] | 9.01×10 ⁻¹ |
| serotonin | Amino acid | -0.00 [-0.05:0.04] | 9.04×10 ⁻¹ |
| acetylcarnitine | Lipid | -0.00 [-0.04:0.04] | 9.04×10 ⁻¹ |
| isobutyrylcarnitine | Amino acid | 0.00 [-0.04:0.04] | 9.05×10 ⁻¹ |
| HWESASXX | Peptide | -0.00 [-0.04:0.03] | 9.10×10 ⁻¹ |
| bilirubin (E,Z or Z,E) | Cofactors and vitamins | 0.00 [-0.04:0.05] | 9.15×10 ⁻¹ |
| metoprolol acid metabolite | Xenobiotics | -0.01 [-0.19:0.18] | 9.24×10 ⁻¹ |
| 1-docosahexaenoylglycerophosphocholine | Lipid | 0.00 [-0.04:0.04] | 9.37×10 ⁻¹ |
| ergothioneine | Xenobiotics | -0.00 [-0.05:0.05] | 9.38×10 ⁻¹ |
| p-cresol sulfate | Amino acid | 0.00 [-0.04:0.04] | 9.41×10 ⁻¹ |
| indolepropionate | Amino acid | 0.00 [-0.04:0.04] | 9.42×10 ⁻¹ |
| choline | Lipid | 0.00 [-0.04:0.04] | 9.43×10 ⁻¹ |
| isovalerylcarnitine | Amino acid | -0.00 [-0.04:0.04] | 9.45×10 ⁻¹ |
| 2-linoleoylglycerophosphocholine | Lipid | -0.00 [-0.04:0.04] | 9.46×10 ⁻¹ |
| docosapentaenoate (n3 DPA; 22:5n3) | Lipid | 0.00 [-0.04:0.04] | 9.47×10 ⁻¹ |

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| 1-palmitoylglycerophosphocholine | Lipid | -0.00 [-0.04:0.04] | 9.50×10^{-1} |
| phosphate | Energy | -0.00 [-0.04:0.04] | 9.53×10^{-1} |
| phenylacetylglutamine | Amino acid | 0.00 [-0.04:0.04] | 9.60×10^{-1} |
| 3-methylxanthine | Xenobiotics | 0.00 [-0.04:0.05] | 9.61×10^{-1} |
| DSGEGDFXAEGGGVR | Peptide | -0.00 [-0.05:0.05] | 9.62×10^{-1} |
| xanthine | Nucleotide | -0.00 [-0.04:0.04] | 9.80×10^{-1} |
| gamma-glutamylglutamine | Peptide | -0.00 [-0.04:0.04] | 9.99×10^{-1} |