

Supplementary materials

Vertical metabolome transfer from mother to child: an explainable machine learning method for detecting metabolomic heritability

Mario Lovric, David Horner, Liang Chen, Nicklas Brustad, Ann-Marie Malby Schoos, Jessica Lasky-Su, Bo Chawes, Morten Arendt Rasmussen

Table S1. List of metabolites which entered the models (N=679).

| | Column1 | Column2 | Column3 | Column4 |
|----|--|--|---|---|
| 0 | linoleate (18:2n6)_Long Chain Polyunsaturated Fatty Acid (n3 and n6)_Lipid | allantoin_Purine Metabolism, (Hypo)Xanthine/Inosine containing_Nucleotide | arachidonate (20:4n6)_Long Chain Polyunsaturated Fatty Acid (n3 and n6)_Lipid | arachidate (20:0)_Long Chain Saturated Fatty Acid_Lipid |
| 1 | myo-inositol_Inositol Metabolism_Lipid | isoleucine_Leucine, Isoleucine and Valine Metabolism_Amino Acid | alanine_Alanine and Aspartate Metabolism_Amino Acid | 3-methoxytyrosine_Tyrosine Metabolism_Amino Acid |
| 2 | beta-hydroxyisovalerate_Leucine, Isoleucine and Valine Metabolism_Amino Acid | threonine_Glycine, Serine and Threonine Metabolism_Amino Acid | tyrosine_Tyrosine Metabolism_Amino Acid | lysine_Lysine Metabolism_Amino Acid |
| 3 | methionine_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid | malate_TCA Cycle_Energy | nonadecanoate (19:0)_Long Chain Saturated Fatty Acid_Lipid | stearate (18:0)_Long Chain Saturated Fatty Acid_Lipid |
| 4 | pentadecanoate (15:0)_Long Chain Saturated Fatty Acid_Lipid | myristate (14:0)_Long Chain Saturated Fatty Acid_Lipid | kynurenate_Tryptophan Metabolism_Amino Acid | 5,6-dihydrothymine_Pyrimidine Metabolism, Thymine containing_Nucleotide |
| 5 | 5-methylthioadenosine (MTA)_Polyamine Metabolism_Amino Acid | succinate_TCA Cycle_Energy | ornithine_Urea cycle; Arginine and Proline Metabolism_Amino Acid | 5-oxoproline_Glutathione Metabolism_Amino Acid |
| 6 | N6,N6,N6-trimethyllysine_Lysine Metabolism_Amino Acid | pantothenate (Vitamin B5)_Pantothenate and CoA Metabolism_Cofactors and Vitamins | picolinate_Tryptophan Metabolism_Amino Acid | glycerol_Glycerolipid Metabolism_Lipid |
| 7 | kynurenine_Tryptophan Metabolism_Amino Acid | sarcosine_Glycine, Serine and Threonine Metabolism_Amino Acid | tartarate_Food Component/Plant_Xenobiotics | glucuronate_Aminosugar Metabolism_Carbohydrate |
| 8 | 3-hydroxyisobutyrate_Leucine, Isoleucine and Valine Metabolism_Amino Acid | carnitine_Carnitine Metabolism_Lipid | choline_Phospholipid Metabolism_Lipid | 4-acetamidobutanoate_Polyamine Metabolism_Amino Acid |
| 9 | alpha-tocopherol_Tocopherol Metabolism_Cofactors and Vitamins | chenodeoxycholate_Primary Bile Acid Metabolism_Lipid | citrate_TCA Cycle_Energy | 1-methyladenosine_Purine Metabolism, Adenine containing_Nucleotide |
| 10 | 3-aminoisobutyrate_Pyrimidine Metabolism, Thymine containing_Nucleotide | vanillylmandelate (VMA)_Tyrosine Metabolism_Amino Acid | 3-methyl-2-oxovalerate_Leucine, Isoleucine and Valine Metabolism_Amino Acid | 3-methylhistidine_Histidine Metabolism_Amino Acid |
| 11 | xanthurenate_Tryptophan Metabolism_Amino Acid | 4-guanidinobutanoate_Guanidino and Acetamido Metabolism_Amino Acid | 5-hydroxylysine_Lysine Metabolism_Amino Acid | imidazole lactate_Histidine Metabolism_Amino Acid |
| 12 | glycerate_Glycolysis, Gluconeogenesis, and Pyruvate Metabolism_Carbohydrate | N-acetylglutamate_Glutamate Metabolism_Amino Acid | methylsuccinate_Leucine, Isoleucine and Valine Metabolism_Amino Acid | 3-phenylpropionate (hydrocinnamate)_Benzoate Metabolism_Xenobiotics |

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|----|--|---|--|---|
| 13 | hippurate_Benzoate Metabolism_Xenobiotics | ethylmalonate_Leucine, Isoleucine and Valine Metabolism_Amino Acid | ribitol_Pentose Metabolism_Carbohydrate | N-acetylalanine_Alanine and Aspartate Metabolism_Amino Acid |
| 14 | glycerophosphorylcholine (GPC)_Phospholipid Metabolism_Lipid | phosphoethanolamine (PE)_Phospholipid Metabolism_Lipid | urate_Purine Metabolism, (Hypo)Xanthine/Inosine containing_Nucleotide | arginine_Urea cycle; Arginine and Proline Metabolism_Amino Acid |
| 15 | caprate (10:0)_Medium Chain Fatty Acid_Lipid | fumarate_TCA Cycle_Energy | heptanoate (7:0)_Medium Chain Fatty Acid_Lipid | serine_Glycine, Serine and Threonine Metabolism_Amino Acid |
| 16 | valine_Leucine, Isoleucine and Valine Metabolism_Amino Acid | 4- hydroxyphenylpyruvate_Tyrosi ne Metabolism_Amino Acid | urea_Urea cycle; Arginine and Proline Metabolism_Amino Acid | cortisol_Corticosteroids_Lipi d |
| 17 | cortisone_Corticosteroids_L ipid | sphingosine_Sphingosines_Lipi d | dihomolinoleate (20:2n6)_Long Chain Polyunsaturated Fatty Acid (n3 and n6)_Lipid | 2-hydroxystearate_Fatty Acid, Monohydroxy_Lipid |
| 18 | retinol (Vitamin A)_Vitamin A Metabolism_Cofactors and Vitamins | gamma- glutamylhistidine_Gamma- glutamyl Amino Acid_Peptide | quinat_Food Component/Plant_Xenobioti cs | indolelactate_Tryptophan Metabolism_Amino Acid |
| 19 | azelate (C9-DC)_Fatty Acid, Dicarboxylate_Lipid | cys-gly, oxidized_Glutathione Metabolism_Amino Acid | gamma- glutamylleucine_Gamma- glutamyl Amino Acid_Peptide | methionine sulfoxide_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid |
| 20 | theobromine_Xanthine Metabolism_Xenobiotics | theophylline_Xanthine Metabolism_Xenobiotics | eicosapentaenoate (EPA; 20:5n3)_Long Chain Polyunsaturated Fatty Acid (n3 and n6)_Lipid | glycocholate_Primary Bile Acid Metabolism_Lipid |
| 21 | taurochenodeoxycholate_P rimary Bile Acid Metabolism_Lipid | taurocholate_Primary Bile Acid Metabolism_Lipid | cysteine_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid | proline_Urea cycle; Arginine and Proline Metabolism_Amino Acid |
| 22 | quinolinate_Nicotinate and Nicotinamide Metabolism_Cofactors and Vitamins | 1,2-dipalmitoyl-GPC (16:0/16:0)_Phosphatidylcholin e (PC)_Lipid | 1-myristoyl-2-palmitoyl-GPC (14:0/16:0)_Phosphatidylcholin e (PC)_Lipid | 1-palmitoyl-2-oleoyl-GPE (16:0/18:1)_Phosphatidyleth anolamine (PE)_Lipid |
| 23 | 1-stearoyl-2-oleoyl-GPS (18:0/18:1)_Phosphatidylse rine (PS)_Lipid | 1-stearoyl-GPI (18:0)_Lysophospholipid_Lipid | stearoyl sphingomyelin (d18:1/18:0)_Sphingomyelins _Lipid | 1,5-anhydroglucitol (1,5- AG)_Glycolysis, Gluconeogenesis, and Pyruvate Metabolism_Carbohydrate |
| 24 | maleate_Fatty Acid, Dicarboxylate_Lipid | tartronate (hydroxymalonate)_Food Component/Plant_Xenobiotics | oxalate (ethanedioate)_Ascorbate and Aldarate Metabolism_Cofactors and Vitamins | iminodiacetate (IDA)_Chemical_Xenobiotics |
| 25 | 2-oleoylglycerol (18:1)_Monoacylglycerol_Li pid | taurine_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid | citrulline_Urea cycle; Arginine and Proline Metabolism_Amino Acid | 3-hydroxyoctanoate_Fatty Acid, Monohydroxy_Lipid |
| 26 | 3-hydroxydecanoate_Fatty Acid, Monohydroxy_Lipid | 4-methyl-2- oxopentanoate_Leucine, Isoleucine and Valine Metabolism_Amino Acid | phenyllactate (PLA)_Phenylalanine Metabolism_Amino Acid | alpha- hydroxyisocaproate_Leucine, Isoleucine and Valine Metabolism_Amino Acid |
| 27 | homoarginine_Urea cycle; Arginine and Proline Metabolism_Amino Acid | homocitrulline_Urea cycle; Arginine and Proline Metabolism_Amino Acid | EDTA_Chemical_Xenobiotics | cysteine s- sulfate_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid |
| 28 | gamma- glutamylglutamine_Gamma -glutamyl Amino Acid_Peptide | gamma- glutamyltyrosine_Gamma- glutamyl Amino Acid_Peptide | indoleacetate_Tryptophan Metabolism_Amino Acid | thyroxine_Tyrosine Metabolism_Amino Acid |
| 29 | 1- methylnicotinamide_Nicoti nate and Nicotinamide Metabolism_Cofactors and Vitamins | 3-indoxyl sulfate_Tryptophan Metabolism_Amino Acid | N-acetylglycine_Glycine, Serine and Threonine Metabolism_Amino Acid | creatine_Creatine Metabolism_Amino Acid |

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| 30 | galactonate_Fructose, Mannose and Galactose Metabolism_Carbohydrate | ribonate_Pentose Metabolism_Carbohydrate | threonate_Ascorbate and Aldarate Metabolism_Cofactors and Vitamins | N-formylmethionine_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid |
| 31 | hypoxanthine_Purine Metabolism, (Hypo)Xanthine/Inosine containing_Nucleotide | betaine_Glycine, Serine and Threonine Metabolism_Amino Acid | xanthine_Purine Metabolism, (Hypo)Xanthine/Inosine containing_Nucleotide | N-(2-furoyl)glycine_Food Component/Plant_Xenobiotics |
| 32 | 3-ureidopropionate_Pyrimidine Metabolism, Uracil containing_Nucleotide | androsterone sulfate_Androgenic Steroids_Lipid | 3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)_Fatty Acid, Dicarboxylate_Lipid | 3-(4-hydroxyphenyl)lactate (HPLA)_Tyrosine Metabolism_Amino Acid |
| 33 | acetylcarnitine (C2)_Fatty Acid Metabolism (Acyl Carnitine, Short Chain)_Lipid | hydroxyproline_Urea cycle; Arginine and Proline Metabolism_Amino Acid | hexanoylcarnitine (C6)_Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)_Lipid | glycochenodeoxycholate_Primary Bile Acid Metabolism_Lipid |
| 34 | 4-imidazoleacetate_Histidine Metabolism_Amino Acid | 1-methyl-4-imidazoleacetate_Histidine Metabolism_Amino Acid | N-acetylneuraminate_Aminosugar Metabolism_Carbohydrate | dodecanedioate (C12)_Fatty Acid, Dicarboxylate_Lipid |
| 35 | 3-hydroxy-2-methylpropionate_Leucine, Isoleucine and Valine Metabolism_Amino Acid | trigonelline (N'-methylnicotinate)_Nicotinate and Nicotinamide Metabolism_Cofactors and Vitamins | indolepropionate_Tryptophan Metabolism_Amino Acid | docosadienoate (22:2n6)_Long Chain Polyunsaturated Fatty Acid (n3 and n6)_Lipid |
| 36 | myristoleate (14:1n5)_Long Chain Monounsaturated Fatty Acid_Lipid | dehydroepiandrosterone sulfate (DHEA-S)_Androgenic Steroids_Lipid | propionylcarnitine (C3)_Fatty Acid Metabolism (also BCAA Metabolism)_Lipid | 3-hydroxylaurate_Fatty Acid, Monohydroxy_Lipid |
| 37 | caproate (6:0)_Medium Chain Fatty Acid_Lipid | 10-undecenoate (11:1n1)_Medium Chain Fatty Acid_Lipid | docosapentaenoate (DPA; 22:5n3)_Long Chain Polyunsaturated Fatty Acid (n3 and n6)_Lipid | 2-linoleoylglycerol (18:2)_Monoacylglycerol_Lipid |
| 38 | phenol sulfate_Tyrosine Metabolism_Amino Acid | pregnen-diol disulfate*_Pregnenolone Steroids_Lipid | X - 11261_NA_NA | bilirubin (E,E)*_Hemoglobin and Porphyrin Metabolism_Cofactors and Vitamins |
| 39 | glycochenolate sulfate*_Secondary Bile Acid Metabolism_Lipid | pregnenediol sulfate (C21H34O5S)*_Pregnenolone Steroids_Lipid | glycolithocholate sulfate*_Secondary Bile Acid Metabolism_Lipid | taurochenolate sulfate*_Secondary Bile Acid Metabolism_Lipid |
| 40 | andro steroid monosulfate C19H28O6S (1)*_Androgenic Steroids_Lipid | adrenate (22:4n6)_Long Chain Polyunsaturated Fatty Acid (n3 and n6)_Lipid | X - 11787_NA_NA | X - 11795_NA_NA |
| 41 | 1-arachidonoyl-GPC* (20:4)*_Lysophospholipid_Lipid | 1-palmitoleoyl-GPC* (16:1)*_Lysophospholipid_Lipid | gamma-glutamylthreonine_Gamma-glutamyl Amino Acid_Peptide | gamma-glutamylphenylalanine_Gamma-glutamyl Amino Acid_Peptide |
| 42 | isobutyrylcarnitine (C4)_Leucine, Isoleucine and Valine Metabolism_Amino Acid | pseudouridine_Pyrimidine Metabolism, Uracil containing_Nucleotide | palmitoleate (16:1n7)_Long Chain Monounsaturated Fatty Acid_Lipid | eicosenoate (20:1n9 or 1n11)_Long Chain Monounsaturated Fatty Acid_Lipid |
| 43 | gamma-glutamyl-epsilon-lysine_Gamma-glutamyl Amino Acid_Peptide | piperine_Food Component/Plant_Xenobiotics | N-acetylthreonine_Glycine, Serine and Threonine Metabolism_Amino Acid | decanoylcarnitine (C10)_Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)_Lipid |
| 44 | N-acetylglutamine_Glutamate Metabolism_Amino Acid | N-acetylhistidine_Histidine Metabolism_Amino Acid | gamma-glutamyltryptophan_Gamma-glutamyl Amino Acid_Peptide | gamma-glutamylglycine_Gamma-glutamyl Amino Acid_Peptide |
| 45 | N-acetylphenylalanine_Phenylalanine Metabolism_Amino Acid | myristoylcarnitine (C14)_Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)_Lipid | N-acetylarginine_Urea cycle; Arginine and Proline Metabolism_Amino Acid | 1-palmitoyl-GPC (16:0)_Lysophospholipid_Lipid |

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| 46 | N-acetyltryptophan_Tryptophan Metabolism_Amino Acid | 1-stearoyl-GPC (18:0)_Lysophospholipid_Lipid | 10-nonadecenoate (19:1n9)_Long Chain Monounsaturated Fatty Acid_Lipid | campesterol_Sterol_Lipid |
| 47 | hyocholate_Secondary Bile Acid Metabolism_Lipid | 1-arachidonoyl-GPI* (20:4)*_Lysophospholipid_Lipid | stachydrine_Food Component/Plant_Xenobiotics | phosphocholine_Phospholipid Metabolism_Lipid |
| 48 | isovalerylcarnitine (C5)_Leucine, Isoleucine and Valine Metabolism_Amino Acid | stearoylcarnitine (C18)_Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)_Lipid | 1-linoleoyl-GPC (18:2)_Lysophospholipid_Lipid | 1-palmitoyl-GPA (16:0)_Lysophospholipid_Lipid |
| 49 | sphingosine 1-phosphate_Sphingosines_Lipid | laurylcarnitine (C12)_Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)_Lipid | isovalerylglycine_Leucine, Isoleucine and Valine Metabolism_Amino Acid | 7-methylguanine_Purine Metabolism, Guanine containing_Nucleotide |
| 50 | phenylacetylglutamine_Acetylated Peptides_Peptide | prolylhydroxyproline_Urea cycle; Arginine and Proline Metabolism_Amino Acid | N4-acetylcytidine_Pyrimidine Metabolism, Cytidine containing_Nucleotide | 5-methyluridine (ribothymidine)_Pyrimidine Metabolism, Uracil containing_Nucleotide |
| 51 | N2,N2-dimethylguanosine_Purine Metabolism, Guanine containing_Nucleotide | N6-carbamoylthreonyladenosine_Purine Metabolism, Adenine containing_Nucleotide | oleoylcarnitine (C18)_Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)_Lipid | 1-arachidonoyl-GPE (20:4n6)*_Lysophospholipid_Lipid |
| 52 | 2-palmitoyl-GPC* (16:0)*_Lysophospholipid_Lipid | 1-palmitoyl-GPI* (16:0)_Lysophospholipid_Lipid | catechol sulfate_Benzoate Metabolism_Xenobiotics | tiglyl carnitine (C5)_Leucine, Isoleucine and Valine Metabolism_Amino Acid |
| 53 | isobutyrylglycine (C4)_Leucine, Isoleucine and Valine Metabolism_Amino Acid | 4-hydroxyhippurate_Benzoate Metabolism_Xenobiotics | 1-oleoyl-GPE (18:1)_Lysophospholipid_Lipid | 1-palmitoyl-GPE (16:0)_Lysophospholipid_Lipid |
| 54 | N-acetyl-aspartyl-glutamate (NAAG)_Glutamate Metabolism_Amino Acid | tetradecanedioate (C14)_Fatty Acid, Dicarboxylate_Lipid | hexadecanedioate (C16)_Fatty Acid, Dicarboxylate_Lipid | dihomolinolenate (20:3n3 or 3n6)_Long Chain Polyunsaturated Fatty Acid (n3 and n6)_Lipid |
| 55 | thymol sulfate_Food Component/Plant_Xenobiotics | 4-vinylphenol sulfate_Benzoate Metabolism_Xenobiotics | 4-ethylphenyl sulfate_Benzoate Metabolism_Xenobiotics | p-cresol sulfate_Benzoate Metabolism_Xenobiotics |
| 56 | 1-linoleoyl-GPI* (18:2)*_Lysophospholipid_Lipid | 1-linoleoyl-GPE (18:2)*_Lysophospholipid_Lipid | 1-oleoyl-GPI (18:1)_Lysophospholipid_Lipid | gamma-glutamylglutamate_Gamma-glutamyl Amino Acid_Peptide |
| 57 | 2-hydroxy-3-methylvalerate_Leucine, Isoleucine and Valine Metabolism_Amino Acid | deoxycarnitine_Carnitine Metabolism_Lipid | N6-acetyllysine_Lysine Metabolism_Amino Acid | octadecanedioate (C18)_Fatty Acid, Dicarboxylate_Lipid |
| 58 | 7-HOCA_Sterol_Lipid | dimethylarginine (ADMA + SDMA)_Urea cycle; Arginine and Proline Metabolism_Amino Acid | tauroolithocholate 3-sulfate_Secondary Bile Acid Metabolism_Lipid | succinylcarnitine (C4-DC)_TCA Cycle_Energy |
| 59 | gamma-glutamylalanine_Gamma-glutamyl Amino Acid_Peptide | N-acetylserine_Glycine, Serine and Threonine Metabolism_Amino Acid | gamma-glutamyl-2-aminobutyrate_Gamma-glutamyl Amino Acid_Peptide | tryptophan betaine_Tryptophan Metabolism_Amino Acid |
| 60 | 4-allylphenol sulfate_Food Component/Plant_Xenobiotics | 5alpha-pregnan-3beta,20alpha-diol disulfate_Progestin Steroids_Lipid | 5alpha-pregnan-3beta,20alpha-diol monosulfate (2)_Progestin Steroids_Lipid | androstenediol (3beta,17beta) disulfate (1)_Androgenic Steroids_Lipid |
| 61 | androstenediol (3beta,17beta) disulfate (2)_Androgenic Steroids_Lipid | androstenediol (3alpha,17alpha) monosulfate (3)_Androgenic Steroids_Lipid | N-acetyl-beta-alanine_Pyrimidine Metabolism, Uracil containing_Nucleotide | glycerophosphoethanolamine_Phospholipid Metabolism_Lipid |
| 62 | ergothioneine_Food Component/Plant_Xenobiotics | docosapentaenoate (n6 DPA; 22:5n6)_Long Chain Polyunsaturated Fatty Acid (n3 and n6)_Lipid | N-acetylputrescine_Polyamine Metabolism_Amino Acid | palmitoyl sphingomyelin (d18:1/16:0)_Sphingomyelin_Lipid |

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| 63 | sphingomyelin (d18:1/18:1, d18:2/18:0)_Sphingomyelins_Lipid | 13-HODE + 9-HODE_Fatty Acid, Monohydroxy_Lipid | 4-cholesten-3-one_Sterol_Lipid | 16a-hydroxy DHEA 3-sulfate_Androgenic Steroids_Lipid |
| 64 | pregnenolone sulfate_Pregnenolone Steroids_Lipid | cis-4-decenoylcarnitine (C10:1)_Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)_Lipid | pristanate_Fatty Acid, Branched_Lipid | 2,3-dihydroxyisovalerate_Food Component/Plant_Xenobiotics |
| 65 | (16 or 17)-methylstearate (a19:0 or i19:0)_Fatty Acid, Branched_Lipid | 12,13-DiHOME_Fatty Acid, Dihydroxy_Lipid | 9,10-DiHOME_Fatty Acid, Dihydroxy_Lipid | cinnamoylglycine_Food Component/Plant_Xenobiotics |
| 66 | (14 or 15)-methylpalmitate (a17:0 or i17:0)_Fatty Acid, Branched_Lipid | 1-(1-enyl-palmitoyl)-GPE (P-16:0)*_Lysoplasmalogen_Lipid | 1-(1-enyl-stearoyl)-GPE (P-18:0)*_Lysoplasmalogen_Lipid | glycoursodeoxycholate_Secondary Bile Acid Metabolism_Lipid |
| 67 | S-methylcysteine_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid | glutarate (C5-DC)_Fatty Acid, Dicarboxylate_Lipid | 16-hydroxypalmitate_Fatty Acid, Monohydroxy_Lipid | eicosanedioate (C20-DC)_Fatty Acid, Dicarboxylate_Lipid |
| 68 | docosadioate (C22-DC)_Fatty Acid, Dicarboxylate_Lipid | carboxyethyl-GABA_Glutamate Metabolism_Amino Acid | isoleucylglycine_Dipeptide_Peptide | 4-hydroxy-2-oxoglutaric acid_Fatty Acid, Dicarboxylate_Lipid |
| 69 | trimethylamine N-oxide_Phospholipid Metabolism_Lipid | N1-Methyl-2-pyridone-5-carboxamide_Nicotinate and Nicotinamide Metabolism_Cofactors and Vitamins | hydantoin-5-propionate_Histidine Metabolism_Amino Acid | 4-hydroxyglutamate_Glutamate Metabolism_Amino Acid |
| 70 | butyrate/isobutyrate (4:0)_Short Chain Fatty Acid_Lipid | 2-stearoyl-GPE (18:0)*_Lysophospholipid_Lipid | lanthionine_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid | N-palmitoylglycine_Fatty Acid Metabolism (Acyl Glycine)_Lipid |
| 71 | phosphate_Oxidative Phosphorylation_Energy | 5-1-pyrroline-5-carboxylate_Glutamate Metabolism_Amino Acid | 2-aminobutyrate_Glutathione Metabolism_Amino Acid | 1-stearoyl-GPE (18:0)_Lysophospholipid_Lipid |
| 72 | erythronate*_Aminosugar Metabolism_Carbohydrate | 1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)_Phosphatidylcholine (PC)_Lipid | 1-stearoyl-2-oleoyl-GPE (18:0/18:1)_Phosphatidylethanolamine (PE)_Lipid | 1-palmitoyl-2-linoleoyl-GPE (16:0/18:2)_Phosphatidylethanolamine (PE)_Lipid |
| 73 | 1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)_Phosphatidylcholine (PC)_Lipid | sphingomyelin (d18:2/16:0, d18:1/16:1)*_Sphingomyelins_Lipid | sphingomyelin (d18:1/14:0, d16:1/16:0)*_Sphingomyelins_Lipid | 2-hydroxydecanoate_Fatty Acid, Monohydroxy_Lipid |
| 74 | glycorychololate_Secondary Bile Acid Metabolism_Lipid | 6-oxopiperidine-2-carboxylate_Lysine Metabolism_Amino Acid | 2-aminophenol sulfate_Chemical_Xenobiotics | 2-aminooctanoate_Fatty Acid, Amino_Lipid |
| 75 | S-methylcysteine sulfoxide_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid | 2-piperidinone_Food Component/Plant_Xenobiotics | dimethyl sulfone_Chemical_Xenobiotics | N-acetylcarnosine_Histidine Metabolism_Amino Acid |
| 76 | formiminoglutamate_Histidine Metabolism_Amino Acid | N-formylanthranilic acid_Tryptophan Metabolism_Amino Acid | 5-(galactosylhydroxy)-L-lysine_Lysine Metabolism_Amino Acid | 2-aminoheptanoate_Fatty Acid, Amino_Lipid |
| 77 | guanidinoacetate_Creatine Metabolism_Amino Acid | bilirubin_Hemoglobin and Porphyrin Metabolism_Cofactors and Vitamins | gamma-glutamylvaline_Gamma-glutamyl Amino Acid_Peptide | glycerol 3-phosphate_Glycerolipid Metabolism_Lipid |
| 78 | 3-methyl-2-oxobutyrate_Leucine, Isoleucine and Valine Metabolism_Amino Acid | 1-(1-enyl-oleoyl)-GPE (P-18:1)*_Lysoplasmalogen_Lipid | isovalerate (C5)_Leucine, Isoleucine and Valine Metabolism_Amino Acid | glutaryl carnitine (C5-DC)_Lysine Metabolism_Amino Acid |
| 79 | palmitoylcarnitine (C16)_Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)_Lipid | gamma-glutamylmethionine_Gamma-glutamyl Amino Acid_Peptide | gamma-CEHC_Tocopherol Metabolism_Cofactors and Vitamins | N-palmitoyl-sphingosine (d18:1/16:0)_Ceramides_Lipid |
| 80 | methionine sulfone_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid | 2-methylbutyrylcarnitine (C5)_Leucine, Isoleucine and Valine Metabolism_Amino Acid | O-sulfo-L-tyrosine_Chemical_Xenobiotics | 1-linolenoyl-GPC (18:3)*_Lysophospholipid_Lipid |

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| 81 | 1-oleoyl-GPG (18:1)*_Lysophospholipid_L lipid | 1-palmitoyl-GPG (16:0)*_Lysophospholipid_L lipid | guaiacol sulfate_Benzoate Metabolism_Xenobiotics | 21-hydroxypregnenolone disulfate_Pregnenolone Steroids_Lipid |
| 82 | mannitol/sorbitol_Fructose, Mannose and Galactose Metabolism_Carbohydrate | 4-methylcatechol sulfate_Benzoate Metabolism_Xenobiotics | 3-methyl catechol sulfate (1)_Benzoate Metabolism_Xenobiotics | aconitate [cis or trans]_TCA Cycle_Energy |
| 83 | linoleoylcarnitine (C18:2)*_Fatty Acid Metabolism (Acyl Carnitine, Polyunsaturated)_Lipid | pyroglutamine*_Glutamate Metabolism_Amino Acid | X - 21258_NA_NA | X - 15486_NA_NA |
| 84 | X - 15461_NA_NA | X - 21286_NA_NA | X - 21310_NA_NA | X - 11441_NA_NA |
| 85 | X - 21319_NA_NA | X - 21339_NA_NA | X - 11308_NA_NA | X - 21353_NA_NA |
| 86 | X - 21364_NA_NA | X - 13866_NA_NA | X - 21383_NA_NA | X - 21410_NA_NA |
| 87 | X - 11444_NA_NA | X - 21441_NA_NA | X - 21448_NA_NA | X - 11850_NA_NA |
| 88 | X - 21467_NA_NA | X - 21470_NA_NA | X - 21471_NA_NA | alpha- hydroxyisovalerate_Leucine, Isoleucine and Valine Metabolism_Amino Acid |
| 89 | N-acetylglucosamine/N- acetylgalactosamine_Amino sugar Metabolism_Carbohydrate | 3-methylglutaryl carnitine (2)_Leucine, Isoleucine and Valine Metabolism_Amino Acid | X - 11299_NA_NA | X - 11372_NA_NA |
| 90 | X - 11470_NA_NA | X - 11478_NA_NA | X - 11530_NA_NA | X - 11880_NA_NA |
| 91 | X - 12007_NA_NA | X - 12216_NA_NA | X - 12462_NA_NA | X - 12524_NA_NA |
| 92 | X - 12729_NA_NA | X - 12798_NA_NA | X - 14056_NA_NA | X - 12844_NA_NA |
| 93 | X - 15469_NA_NA | X - 13728_NA_NA | X - 14939_NA_NA | X - 15245_NA_NA |
| 94 | X - 16935_NA_NA | X - 16944_NA_NA | X - 16964_NA_NA | X - 18779_NA_NA |
| 95 | X - 18913_NA_NA | X - 18922_NA_NA | X - 19141_NA_NA | X - 17653_NA_NA |
| 96 | X - 17654_NA_NA | X - 21736_NA_NA | X - 12104_NA_NA | gulonate*_Ascorbate and Aldarate Metabolism_Cofactors and Vitamins |
| 97 | sulfate*_Chemical_Xenobio tics | X - 17676_NA_NA | X - 15503_NA_NA | X - 12193_NA_NA |
| 98 | X - 21829_NA_NA | N- methylpipecolate_Bacterial/Fu ngal_Xenobiotics | ferulic acid 4-sulfate_Food Component/Plant_Xenobioti cs | 2-palmitoleoyl-GPC* (16:1)*_Lysophospholipid_Li pid |
| 99 | 9-hydroxystearate_Fatty Acid, Monohydroxy_Lipid | sphingomyelin (d18:1/24:1, d18:2/24:0)*_Sphingomyelins_ Lipid | sphingomyelin (d18:2/14:0, d18:1/14:1)*_Sphingomyelin s_Lipid | X - 18887_NA_NA |
| 100 | X - 22162_NA_NA | X - 12680_NA_NA | X - 12101_NA_NA | X - 18899_NA_NA |
| 101 | X - 18921_NA_NA | X - 12100_NA_NA | X - 12112_NA_NA | X - 13431_NA_NA |
| 102 | X - 16397_NA_NA | X - 16580_NA_NA | bilirubin (E,Z or Z,E)*_Hemoglobin and Porphyrin Metabolism_Cofactors and Vitamins | X - 12026_NA_NA |
| 103 | X - 12221_NA_NA | X - 12906_NA_NA | X - 13553_NA_NA | X - 17351_NA_NA |
| 104 | X - 17357_NA_NA | X - 22771_NA_NA | mannose_Fructose, Mannose and Galactose Metabolism_Carbohydrate | myristoleoylcarnitine (C14:1)*_Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)_Lipid |
| 105 | N- acetyltaurine_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid | fructose_Fructose, Mannose and Galactose Metabolism_Carbohydrate | arabonate/xylonate_Pentose Metabolism_Carbohydrate | 1-oleoyl-GPC (18:1)_Lysophospholipid_Lipi d |
| 106 | 1-dihomo-linolenylglycerol (20:3)_Monoacylglycerol_Li pid | N1-methylinosine_Purine Metabolism, (Hypo)Xanthine/Inosine containing_Nucleotide | dopamine 3-O- sulfate_Tyrosine Metabolism_Amino Acid | tyramine O-sulfate_Tyrosine Metabolism_Amino Acid |
| 107 | pyrraline_Food Component/Plant_Xenobioti cs | 4- hydroxychlorothalonil_Chemica l_Xenobiotics | 4-vinylguaiacol sulfate_Food Component/Plant_Xenobioti cs | 3-hydroxypyridine sulfate_Chemical_Xenobiotic s |

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|-----|---|--|---|---|
| 108 | 4-methoxyphenol sulfate_Tyrosine Metabolism_Amino Acid | sphingomyelin (d18:1/20:0, d16:1/22:0)*_Sphingomyelins_Lipid | sphingomyelin (d18:1/20:1, d18:2/20:0)*_Sphingomyelins_Lipid | behenoyl sphingomyelin (d18:1/22:0)*_Sphingomyelins_Lipid |
| 109 | sphingomyelin (d18:1/22:1, d18:2/22:0, d16:1/24:1)*_Sphingomyelins_Lipid | 3-methoxycatechol sulfate (1)_Benzoate Metabolism_Xenobiotics | C-glycosyltryptophan_Tryptophan Metabolism_Amino Acid | glycerophosphoglycerol_Glycerolipid Metabolism_Lipid |
| 110 | arabitol/xylitol_Pentose Metabolism_Carbohydrate | X - 23593_NA_NA | X - 23636_NA_NA | X - 23639_NA_NA |
| 111 | X - 23665_NA_NA | X - 23666_NA_NA | X - 23680_NA_NA | X - 11315_NA_NA |
| 112 | 1-lignoceroyl-GPC (24:0)_Lysophospholipid_Lipid | X - 23739_NA_NA | alpha-ketobutyrate_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid | X - 23782_NA_NA |
| 113 | dimethylglycine_Glycine, Serine and Threonine Metabolism_Amino Acid | asparagine_Alanine and Aspartate Metabolism_Amino Acid | creatinine_Creatine Metabolism_Amino Acid | X - 23997_NA_NA |
| 114 | glycosyl-N-stearoyl-sphingosine (d18:1/18:0)_Hexosylceramides (HCER)_Lipid | 2-hydroxybutyrate/2-hydroxyisobutyrate_Glutathione Metabolism_Amino Acid | X - 24243_NA_NA | 1-palmitoleoylglycerol (16:1)*_Monoacylglycerol_Lipid |
| 115 | sphingomyelin (d17:1/16:0, d18:1/15:0, d16:1/17:0)*_Sphingomyelins_Lipid | palmitoyl dihydrosphingomyelin (d18:0/16:0)*_Dihydrosphingomyelins_Lipid | sphingomyelin (d18:2/23:0, d18:1/23:1, d17:1/24:1)*_Sphingomyelins_Lipid | tricosanoyl sphingomyelin (d18:1/23:0)*_Sphingomyelins_Lipid |
| 116 | sphingomyelin (d18:2/24:1, d18:1/24:2)*_Sphingomyelins_Lipid | 1-stearoyl-2-oleoyl-GPC (18:0/18:1)_Phosphatidylcholine (PC)_Lipid | 1-stearoyl-2-arachidonoyl-GPE (18:0/20:4)_Phosphatidylethanolamine (PE)_Lipid | 1-stearoyl-2-arachidonoyl-GPI (18:0/20:4)_Phosphatidylinositol (PI)_Lipid |
| 117 | 1-palmitoyl-2-linoleoyl-GPI (16:0/18:2)_Phosphatidylinositol (PI)_Lipid | 1-stearoyl-2-linoleoyl-GPC (18:0/18:2)*_Phosphatidylcholine (PC)_Lipid | 1-palmitoyl-2-oleoyl-GPC (16:0/18:1)_Phosphatidylcholine (PC)_Lipid | 1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4n6)_Phosphatidylcholine (PC)_Lipid |
| 118 | 1-palmitoyl-2-arachidonoyl-GPE (16:0/20:4)*_Phosphatidylethanolamine (PE)_Lipid | 1-palmitoyl-2-docosahexaenoyl-GPE (16:0/22:6)*_Phosphatidylethanolamine (PE)_Lipid | 1-stearoyl-2-docosahexaenoyl-GPE (18:0/22:6)*_Phosphatidylethanolamine (PE)_Lipid | 1-palmitoyl-2-arachidonoyl-GPI (16:0/20:4)*_Phosphatidylinositol (PI)_Lipid |
| 119 | 1-stearoyl-2-linoleoyl-GPI (18:0/18:2)_Phosphatidylinositol (PI)_Lipid | 1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)*_Phosphatidylcholine (PC)_Lipid | gamma-tocopherol/beta-tocopherol_Tocopherol Metabolism_Cofactors and Vitamins | 1-(1-enyl-palmitoyl)-GPC (P-16:0)*_Lysoplasmalogen_Lipid |
| 120 | 1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*_Plasmalogen_Lipid | 1-(1-enyl-palmitoyl)-2-oleoyl-GPE (P-16:0/18:1)*_Plasmalogen_Lipid | 1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)*_Plasmalogen_Lipid | X - 24295_NA_NA |
| 121 | sphingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)*_Sphingomyelins_Lipid | X - 24307_NA_NA | X - 24337_NA_NA | 1,2-dilinoeloyl-GPC (18:2/18:2)_Phosphatidylcholine (PC)_Lipid |
| 122 | N-palmitoyl-sphinganine (d18:0/16:0)_Dihydroceramides_Lipid | sphinganine-1-phosphate_Sphingolipid Synthesis_Lipid | 1-palmitoyl-2-docosahexaenoyl-GPC (16:0/22:6)_Phosphatidylcholine (PC)_Lipid | 1-stearoyl-2-docosahexaenoyl-GPC (18:0/22:6)_Phosphatidylcholine (PC)_Lipid |
| 123 | 1-(1-enyl-stearoyl)-2-oleoyl-GPE (P-18:0/18:1)_Plasmalogen_Lipid | sphingomyelin (d18:1/17:0, d17:1/18:0, d19:1/16:0)_Sphingomyelins_Lipid | 1-palmitoyl-2-stearoyl-GPC (16:0/18:0)_Phosphatidylcholine (PC)_Lipid | X - 24431_NA_NA |
| 124 | X - 24432_NA_NA | 1-palmitoyl-2-oleoyl-GPI (16:0/18:1)*_Phosphatidylinositol (PI)_Lipid | 1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)*_Plasmalogen_Lipid | 1-(1-enyl-palmitoyl)-2-linoleoyl-GPE (P-16:0/18:2)*_Plasmalogen_Lipid |
| 125 | 1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P- | 1-oleoyl-2-linoleoyl-GPE (18:1/18:2)*_Phosphatidylethanolamine (PE)_Lipid | 1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC (P- | 1-linoleoyl-GPA (18:2)*_Lysophospholipid_Lipid |

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|-----|--|--|--|--|
| | 16:0/18:2)*_Plasmalogen_Lipid | | 16:0/20:4)*_Plasmalogen_Lipid | |
| 126 | 1-oleoyl-2-docosa-hexaenoyl-GPC (18:1/22:6)*_Phosphatidylcholine (PC)_Lipid | lactate_Glycolysis, Gluconeogenesis, and Pyruvate Metabolism_Carbohydrate | 1-linoleoyl-2-arachidonoyl-GPC (18:2/20:4n6)*_Phosphatidylcholine (PC)_Lipid | 1-(1-enyl-palmitoyl)-2-palmitoleoyl-GPC (P-16:0/16:1)*_Plasmalogen_Lipid |
| 127 | 1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)*_Plasmalogen_Lipid | 1-stearoyl-2-oleoyl-GPI (18:0/18:1)*_Phosphatidylinositol (PI)_Lipid | 1-(1-enyl-stearoyl)-2-linoleoyl-GPE (P-18:0/18:2)*_Plasmalogen_Lipid | X - 24455_NA_NA |
| 128 | X - 24473_NA_NA | alpha-ketoglutarate_TCA Cycle_Energy | X - 24544_NA_NA | X - 24545_NA_NA |
| 129 | X - 24556_NA_NA | X - 24588_NA_NA | 2-hydroxylaurate_Fatty Acid, Monohydroxy_Lipid | palmitoylcholine_Fatty Acid Metabolism (Acyl Choline)_Lipid |
| 130 | glycochenodeoxycholate 3-sulfate_Primary Bile Acid Metabolism_Lipid | glycodeoxycholate 3-sulfate_Secondary Bile Acid Metabolism_Lipid | glycochenodeoxycholate glucuronide (1)_Primary Bile Acid Metabolism_Lipid | (S)-3-hydroxybutyrylcarnitine_Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)_Lipid |
| 131 | N1,N12-diacetylspermine_Polyamine Metabolism_Amino Acid | adipoylcarnitine (C6-DC)_Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)_Lipid | glutamine_Glutamate Metabolism_Amino Acid | lactosyl-N-palmitoyl-sphingosine (d18:1/16:0)_Lactosylceramides (LCER)_Lipid |
| 132 | glycosyl-N-palmitoyl-sphingosine (d18:1/16:0)_Hexosylceramides (HCER)_Lipid | 3-hydroxy-3-methylglutarate_Mevalonate Metabolism_Lipid | X - 24728_NA_NA | 1-linoleoyl-2-linolenoyl-GPC (18:2/18:3)*_Phosphatidylcholine (PC)_Lipid |
| 133 | 1-palmitoleoyl-2-linolenoyl-GPC (16:1/18:3)*_Phosphatidylcholine (PC)_Lipid | 1-myristoyl-2-arachidonoyl-GPC (14:0/20:4)*_Phosphatidylcholine (PC)_Lipid | palmitoleoylcarnitine (C16:1)*_Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)_Lipid | pimeloylcarnitine/3-methyladipoylcarnitine (C7-DC)_Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)_Lipid |
| 134 | 3-hydroxyhexanoate_Fatty Acid, Monohydroxy_Lipid | thioprolin_Chemical_Xenobiotics | caffeic acid sulfate_Food Component/Plant_Xenobiotics | tryptophan_Tryptophan Metabolism_Amino Acid |
| 135 | 3-hydroxybutyrate (BHBA)_Ketone Bodies_Lipid | 3beta-hydroxy-5-cholestenoate_Sterol_Lipid | 1-linoleoyl-GPG (18:2)*_Lysophospholipid_Lipid | vanillactate_Tyrosine Metabolism_Amino Acid |
| 136 | diacylglycerol (16:1/18:2 [2], 16:0/18:3 [1])*_Diacylglycerol_Lipid | palmitoleoyl-linoleoyl-glycerol (16:1/18:2) [1]*_Diacylglycerol_Lipid | N-stearoyl-sphingosine (d18:1/18:0)*_Ceramides_Lipid | beta-alanine_Pyrimidine Metabolism, Uracil containing_Nucleotide |
| 137 | gamma-glutamyl-alpha-lysine_Gamma-glutamyl Amino Acid_Peptide | 2-oxoarginine*_Urea cycle; Arginine and Proline Metabolism_Amino Acid | phenylpyruvate_Phenylalanine Metabolism_Amino Acid | glutamate_Glutamate Metabolism_Amino Acid |
| 138 | lignoceroyl sphingomyelin (d18:1/24:0)_Sphingomyelins_Lipid | behenoyl dihydrosphingomyelin (d18:0/22:0)*_Dihydrosphingomyelins_Lipid | myristoyl dihydrosphingomyelin (d18:0/14:0)*_Dihydrosphingomyelins_Lipid | lactosyl-N-nervonoyl-sphingosine (d18:1/24:1)*_Lactosylceramides (LCER)_Lipid |
| 139 | N-behenoyl-sphingadienine (d18:2/22:0)*_Ceramides_Lipid | palmitoyl-docosa-hexaenoyl-glycerol (16:0/22:6) [1]*_Diacylglycerol_Lipid | N-palmitoyl-sphingadienine (d18:2/16:0)*_Ceramides_Lipid | lactosyl-N-behenoyl-sphingosine (d18:1/22:0)*_Lactosylceramides (LCER)_Lipid |
| 140 | ceramide (d18:1/14:0, d16:1/16:0)*_Ceramides_Lipid | ceramide (d16:1/24:1, d18:1/22:1)*_Ceramides_Lipid | ceramide (d18:1/20:0, d16:1/22:0, d20:1/18:0)*_Ceramides_Lipid | ceramide (d18:2/24:1, d18:1/24:2)*_Ceramides_Lipid |
| 141 | glycosyl-N-(2-hydroxynervonoyl)-sphingosine (d18:1/24:1(2OH))*_Hexosylceramides (HCER)_Lipid | glycosyl ceramide (d18:2/24:1, d18:1/24:2)*_Hexosylceramides (HCER)_Lipid | argininate*_Urea cycle; Arginine and Proline Metabolism_Amino Acid | sphingomyelin (d18:0/18:0, d19:0/17:0)*_Dihydrosphingomyelins_Lipid |
| 142 | sphingomyelin (d18:2/18:1)*_Sphingomyelins_Lipid | sphingomyelin (d18:1/19:0, d19:1/18:0)*_Sphingomyelins_Lipid | sphingomyelin (d18:1/22:2, d18:2/22:1, | sphingomyelin (d18:1/25:0, d19:0/24:1, d20:1/23:0, |

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|-----|--|---|---|---|
| | | | d16:1/24:2)*_Sphingomyelin s_Lipid | d19:1/24:0)*_Sphingomyelin s_Lipid |
| 143 | sphingomyelin (d18:2/24:2)*_Sphingomyelin s_Lipid | sphingomyelin (d18:2/21:0, d16:2/23:0)*_Sphingomyelin s_Lipid | sphingomyelin (d18:1/20:2, d18:2/20:1, d16:1/22:2)*_Sphingomyelin s_Lipid | sphingomyelin (d17:2/16:0, d18:2/15:0)*_Sphingomyelin s_Lipid |
| 144 | arabinose_Pentose Metabolism_Carbohydrate | margaroylcarnitine (C17)*_Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)_Lipid | arachidoylecarnitine (C20)*_Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)_Lipid | behenoylcarnitine (C22)*_Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)_Lipid |
| 145 | lignoceroylecarnitine (C24)*_Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)_Lipid | cerotoylecarnitine (C26)*_Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)_Lipid | ximenoylcarnitine (C26:1)*_Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)_Lipid | arachidonoylcarnitine (C20:4)_Fatty Acid Metabolism (Acyl Carnitine, Polyunsaturated)_Lipid |
| 146 | eicosenoylcarnitine (C20:1)*_Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)_Lipid | dihomo-linoleoylcarnitine (C20:2)*_Fatty Acid Metabolism (Acyl Carnitine, Polyunsaturated)_Lipid | dihomo-linolenoylcarnitine (C20:3n3 or 6)*_Fatty Acid Metabolism (Acyl Carnitine, Polyunsaturated)_Lipid | nervonoylcarnitine (C24:1)*_Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)_Lipid |
| 147 | 2'-O- methylcytidine_Pyrimidine Metabolism, Cytidine containing_Nucleotide | perfluorooctanesulfonate (PFOS)_Chemical_Xenobiotics | beta-cryptoxanthin_Vitamin A Metabolism_Cofactors and Vitamins | carotene diol (1)_Vitamin A Metabolism_Cofactors and Vitamins |
| 148 | carotene diol (2)_Vitamin A Metabolism_Cofactors and Vitamins | carotene diol (3)_Vitamin A Metabolism_Cofactors and Vitamins | hexadecadienoate (16:2n6)_Long Chain Polyunsaturated Fatty Acid (n3 and n6)_Lipid | N- palmitoylserine_Endocannab inoid_Lipid |
| 149 | 2-hydroxybehenate_Fatty Acid, Monohydroxy_Lipid | N- oleoylserine_Endocannabinoid Lipid | N,N,N-trimethyl-5- aminovalerate_Lysine Metabolism_Amino Acid | X - 24947_NA_NA |
| 150 | X - 24951_NA_NA | 3-methylglutaconate_Leucine, Isoleucine and Valine Metabolism_Amino Acid | X - 24970_NA_NA | nisinate (24:6n3)_Long Chain Polyunsaturated Fatty Acid (n3 and n6)_Lipid |
| 151 | (N(1) + N(8))- acetylspermidine_Polyamin e Metabolism_Amino Acid | glycine_Glycine, Serine and Threonine Metabolism_Amino Acid | gluconate_Food Component/Plant_Xenobioti cs | histidine_Histidine Metabolism_Amino Acid |
| 152 | hypotaurine_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid | phytanate_Food Component/Plant_Xenobiotics | leucine_Leucine, Isoleucine and Valine Metabolism_Amino Acid | dihydroorotate_Pyrimidine Metabolism, Orotate containing_Nucleotide |
| 153 | uridine_Pyrimidine Metabolism, Uracil containing_Nucleotide | trans-urocanate_Histidine Metabolism_Amino Acid | 2-aminoadipate_Lysine Metabolism_Amino Acid | 2-hydroxynervonate*_Fatty Acid, Monohydroxy_Lipid |
| 154 | 2-hydroxyarachidate*_Fatty Acid, Monohydroxy_Lipid | 5,6-dihydrouridine_Pyrimidine Metabolism, Uracil containing_Nucleotide | ribulonate/xylulonate/lyxona te*_Pentose Metabolism_Carbohydrate | octadecadienedioate (C18:2- DC)*_Fatty Acid, Dicarboxylate_Lipid |
| 155 | octadecenedioate (C18:1- DC)_Fatty Acid, Dicarboxylate_Lipid | hexadecenedioate (C16:1- DC)*_Fatty Acid, Dicarboxylate_Lipid | octadecenedioylecarnitine (C18:1-DC)*_Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)_Lipid | heptenedioate (C7:1- DC)*_Fatty Acid, Dicarboxylate_Lipid |
| 156 | octadecanedioylecarnitine (C18-DC)*_Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)_Lipid | 1-ribosyl- imidazoleacetate*_Histidine Metabolism_Amino Acid | 3-carboxy-4-methyl-5-pentyl- 2-furanpropionate (3- CMPFP)_Fatty Acid, Dicarboxylate_Lipid | glucuronide of C12H22O4 (1)*_Partially Characterized Molecules_Partially Characterized Molecules |
| 157 | N-acetyl-2- aminooctanoate*_Fatty Acid, Amino_Lipid | hydroxyasparagine_Alanine and Aspartate Metabolism_Amino Acid | 3-hydroxystachydrine*_Food Component/Plant_Xenobioti cs | glyco-beta- muricholate_Primary Bile Acid Metabolism_Lipid |
| 158 | perfluorooctanoate (PFOA)_Chemical_Xenobioti cs | alpha- ketoglutaminate*_Glutamate Metabolism_Amino Acid | cysteinyglycine disulfide*_Glutathione Metabolism_Amino Acid | gamma- glutamylcitrulline*_Gamma- glutamyl Amino Acid_Peptide |
| 159 | glycine conjugate of C10H14O2 (1)*_Partially Characterized Molecules_Partially Characterized Molecules | X - 25172_NA_NA | sphingomyelin (d17:1/14:0, d16:1/15:0)*_Sphingomyelin s_Lipid | dodecadienoate (12:2)*_Fatty Acid, Dicarboxylate_Lipid |

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|-----|---|--|---|---|
| 160 | hydroxy-CMPF*_Fatty Acid, Dicarboxylate_Lipid | indoleacetyl carnitine*_Tryptophan Metabolism_Amino Acid | N-acetyl-isoputrescine_Polyamine Metabolism_Amino Acid | 1-carboxyethylvaline_Leucine, Isoleucine and Valine Metabolism_Amino Acid |
| 161 | 1-carboxyethylphenylalanine Phenylalanine Metabolism_Amino Acid | 2,3-dihydroxy-5-methylthio-4-pentenoate (DMTPA)*_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid | tetradecadienoate (14:2)*_Long Chain Polyunsaturated Fatty Acid (n3 and n6)_Lipid | hydroxypalmitoyl sphingomyelin (d18:1/16:0(OH))_Sphingomyelins_Lipid |
| 162 | 3-amino-2-piperidone_Urea cycle; Arginine and Proline Metabolism_Amino Acid | N6-methyllysine_Lysine Metabolism_Amino Acid | N6,N6-dimethyllysine_Lysine Metabolism_Amino Acid | cis-4-decenoate (10:1n6)*_Medium Chain Fatty Acid_Lipid |
| 163 | taurochenodeoxycholic acid 3-sulfate_Secondary Bile Acid Metabolism_Lipid | tridecenedioate (C13:1-DC)*_Fatty Acid, Dicarboxylate_Lipid | pregnenetriol disulfate*_Pregnenolone Steroids_Lipid | pregnenetriol sulfate*_Pregnenolone Steroids_Lipid |
| 164 | eicosenedioate (C20:1-DC)*_Fatty Acid, Dicarboxylate_Lipid | 1-methyl-5-imidazoleacetate_Histidine Metabolism_Amino Acid | hydroxy-N6,N6,N6-trimethyllysine*_Lysine Metabolism_Amino Acid | palmitoyl-sphingosine-phosphoethanolamine (d18:1/16:0)_Ceramide PEs_Lipid |
| 165 | cholesterol_Sterol_Lipid | 2,6-dihydroxybenzoic acid_Drug - Topical Agents_Xenobiotics | picolinoylglycine_Fatty Acid Metabolism (Acyl Glycine)_Lipid | N,N-dimethylalanine_Alanine and Aspartate Metabolism_Amino Acid |
| 166 | ethyl alpha-glucopyranoside_Food Component/Plant_Xenobiotics | metabolonic lactone sulfate_Partially Characterized Molecules_Partially Characterized Molecules | branched chain 14:0 dicarboxylic acid_Fatty Acid, Dicarboxylate_Lipid | (2 or 3)-decenoate (10:1n7 or n8)_Medium Chain Fatty Acid_Lipid |
| 167 | 3-indoleglyoxylic acid_Food Component/Plant_Xenobiotics | deoxycholic acid glucuronide_Secondary Bile Acid Metabolism_Lipid | undecenoylcarnitine (C11:1)_Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)_Lipid | branched-chain, straight-chain, or cyclopropyl 10:1 fatty acid (1)*_Partially Characterized Molecules_Partially Characterized Molecules |
| 168 | branched-chain, straight-chain, or cyclopropyl 10:1 fatty acid (2)*_Partially Characterized Molecules_Partially Characterized Molecules | glutamine conjugate of C6H10O2 (1)*_Partially Characterized Molecules_Partially Characterized Molecules | branched-chain, straight-chain, or cyclopropyl 12:1 fatty acid*_Partially Characterized Molecules_Partially Characterized Molecules | vanillic acid glycine_Food Component/Plant_Xenobiotics |
| 169 | 4-chlorobenzoic acid_Chemical_Xenobiotics | 2-O-methylascorbic acid_Ascorbate and Aldarate Metabolism_Cofactors and Vitamins | phenylalanine_Phenylalanine Metabolism_Amino Acid | linoleate (18:2n6)_Long Chain Polyunsaturated Fatty Acid (n3 and n6)_Lipid |

Table S2. The list of 205 metabolites out of the 884, which didn't enter the models.

| | Column1 | Column2 | Column3 | Column4 |
|----|---|--|---|--|
| 0 | inosine_Purine Metabolism, (Hypo)Xanthine/Inosine containing_Nucleotide | 4-allylcatechol sulfate_Benzoate Metabolism_Xenobiotics | X - 16124_NA_NA | X - 25217_NA_NA |
| 1 | X - 21752_NA_NA | hexanoylglutamine_Fatty Acid Metabolism (Acyl Glutamine)_Lipid | cysteine-glutathione disulfide_Glutathione Metabolism_Amino Acid | 5alpha-pregnan-diol disulfate_Progestin Steroids_Lipid |
| 2 | 3-hydroxyhippurate_Benzoate Metabolism_Xenobiotics | 4-acetamidophenylglucuronide_Drug - Analgesics, Anesthetics_Xenobiotics | androsterone glucuronide_Androgenic Steroids_Lipid | xylose_Pentose Metabolism_Carbohydrate |
| 3 | X - 11843_NA_NA | 2-acetamidophenol sulfate_Drug - Analgesics, Anesthetics_Xenobiotics | N,N,N-trimethyl-alanylproline betaine (TMAP)_Urea cycle; Arginine and Proline Metabolism_Amino Acid | X - 24546_NA_NA |
| 4 | androstenediol (3alpha, 17alpha) monosulfate (2)_Androgenic Steroids_Lipid | linoleoylcholine*_Fatty Acid Metabolism (Acyl Choline)_Lipid | docosahexaenoylcholine_Fatty Acid Metabolism (Acyl Choline)_Lipid | X - 12544_NA_NA |
| 5 | solanidine_Food Component/Plant_Xenobiotics | acesulfame_Food Component/Plant_Xenobiotics | cytosine_Pyrimidine Metabolism, Cytidine containing_Nucleotide | nonanoylcarnitine (C9)_Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)_Lipid |
| 6 | X - 17185_NA_NA | X - 12812_NA_NA | 1,2-dilinoeloyl-GPE (18:2/18:2)*_Phosphatidylethanolamine (PE)_Lipid | X - 21796_NA_NA |
| 7 | X - 13684_NA_NA | palmitate (16:0)_Long Chain Saturated Fatty Acid_Lipid | 1,3,7-trimethylurate_Xanthine Metabolism_Xenobiotics | sphingadienine_Sphingolipid Synthesis_Lipid |
| 8 | X - 15728_NA_NA | gentisate_Tyrosine Metabolism_Amino Acid | 4-ethylcatechol sulfate_Benzoate Metabolism_Xenobiotics | 2-ketocaprylate_Leucine, Isoleucine and Valine Metabolism_Amino Acid |
| 9 | X - 12849_NA_NA | glucuronide of C10H18O2 (7)*_Partially Characterized Molecules_Partially Characterized Molecules | linolenate (18:3n3 or 3n6)_Long Chain Polyunsaturated Fatty Acid (n3 and n6)_Lipid | X - 21834_NA_NA |
| 10 | 3-methoxycatechol sulfate (2)_Benzoate Metabolism_Xenobiotics | orotate_Pyrimidine Metabolism, Orotate containing_Nucleotide | X - 17612_NA_NA | 10-heptadecenoate (17:1n7)_Long Chain Monounsaturated Fatty Acid_Lipid |
| 11 | X - 21742_NA_NA | X - 24849_NA_NA | margarate (17:0)_Long Chain Saturated Fatty Acid_Lipid | octanoylcarnitine (C8)_Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)_Lipid |
| 12 | X - 17343_NA_NA | X - 24571_NA_NA | suberate (C8-DC)_Fatty Acid, Dicarboxylate_Lipid | stearoylcholine*_Fatty Acid Metabolism (Acyl Choline)_Lipid |
| 13 | nicotinamide_Nicotinate and Nicotinamide Metabolism_Cofactors and Vitamins | glycoursodeoxycholic acid sulfate (1)_Secondary Bile Acid Metabolism_Lipid | syringol sulfate_Food Component/Plant_Xenobiotics | glucuronide of piperine metabolite C17H21NO3 (4)*_Food Component/Plant_Xenobiotics |
| 14 | X - 24699_NA_NA | tauroursodeoxycholate_Secondary Bile Acid Metabolism_Lipid | eugenol sulfate_Food Component/Plant_Xenobiotics | lithocholate sulfate (1)_Secondary Bile Acid Metabolism_Lipid |
| 15 | 1-stearoyl-2-linoleoyl-GPE (18:0/18:2)*_Phosphatidylethanolamine (PE)_Lipid | 5-acetylamin-6-amino-3-methyluracil_Xanthine Metabolism_Xenobiotics | phenylacetylcarnitine_Acetylated Peptides_Peptide | umbelliferone sulfate_Food Component/Plant_Xenobiotics |
| 16 | X - 24549_NA_NA | 3-methylxanthine_Xanthine Metabolism_Xenobiotics | oleate/vaccenate (18:1)_Long Chain Monounsaturated Fatty Acid_Lipid | 3-(3-hydroxyphenyl)propionate_Benzoate Metabolism_Xenobiotics |

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| 17 | taurohyocholate*_Secondary Bile Acid Metabolism_Lipid | imidazole propionate_Histidine Metabolism_Amino Acid | N-acetylleucine_Leucine, Isoleucine and Valine Metabolism_Amino Acid | X - 21607_NA_NA |
| 18 | 6-hydroxyindole sulfate_Chemical_Xenobiotics | o-cresol sulfate_Benzoate Metabolism_Xenobiotics | deoxycholate_Secondary Bile Acid Metabolism_Lipid | sebacate (C10-DC)_Fatty Acid, Dicarboxylate_Lipid |
| 19 | hydroquinone sulfate_Drug - Topical Agents_Xenobiotics | X - 21803_NA_NA | X - 11442_NA_NA | dihydroferulate_Food Component/Plant_Xenobiotics |
| 20 | erythritol_Food Component/Plant_Xenobiotics | linolenoylcarnitine (C18:3)*_Fatty Acid Metabolism (Acyl Carnitine, Polyunsaturated)_Lipid | 1,7-dimethylurate_Xanthine Metabolism_Xenobiotics | suberoylcarnitine (C8-DC)_Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)_Lipid |
| 21 | cysteinylglycine_Glutathione Metabolism_Amino Acid | 5alpha-pregnan-3beta,20beta-diol monosulfate (1)_Progesterin Steroids_Lipid | maltose_Glycogen Metabolism_Carbohydrate | X - 11858_NA_NA |
| 22 | 1-methylxanthine_Xanthine Metabolism_Xenobiotics | 3,4-methyleneheptanoate_Food Component/Plant_Xenobiotics | ADSGEGDFXAEAGGVR*_Fibrinogen Cleavage Peptide_Peptide | caffeine_Xanthine Metabolism_Xenobiotics |
| 23 | sphinganine_Sphingolipid Synthesis_Lipid | ursodeoxycholate_Secondary Bile Acid Metabolism_Lipid | X - 12411_NA_NA | N-acetyl-1-methylhistidine*_Histidine Metabolism_Amino Acid |
| 24 | 5alpha-androstan-3beta,17alpha-diol disulfate_Androgenic Steroids_Lipid | 2-hydroxypalmitate_Fatty Acid, Monohydroxy_Lipid | X - 23641_NA_NA | chiro-inositol_Inositol Metabolism_Lipid |
| 25 | epiandrosterone sulfate_Androgenic Steroids_Lipid | X - 21442_NA_NA | cholate_Primary Bile Acid Metabolism_Lipid | N-ethylglycinexylidide_Drug - Analgesics, Anesthetics_Xenobiotics |
| 26 | serotonin_Tryptophan Metabolism_Amino Acid | alliin_Food Component/Plant_Xenobiotics | glycodeoxycholate_Secondary Bile Acid Metabolism_Lipid | X - 11522_NA_NA |
| 27 | aspartate_Alanine and Aspartate Metabolism_Amino Acid | AMP_Purine Metabolism, Adenine containing_Nucleotide | dihomo-linolenoyl-choline_Fatty Acid Metabolism (Acyl Choline)_Lipid | X - 11849_NA_NA |
| 28 | 2-hydroxyhippurate (salicylurate)_Benzoate Metabolism_Xenobiotics | methyl glucopyranoside (alpha + beta)_Food Component/Plant_Xenobiotics | 2-hydroxyacetaminophen sulfate*_Drug - Analgesics, Anesthetics_Xenobiotics | docosahexaenoylcarnitine (C22:6)*_Fatty Acid Metabolism (Acyl Carnitine, Polyunsaturated)_Lipid |
| 29 | p-cresol glucuronide*_Tyrosine Metabolism_Amino Acid | paraxanthine_Xanthine Metabolism_Xenobiotics | N-methylproline_Urea cycle; Arginine and Proline Metabolism_Amino Acid | X - 18901_NA_NA |
| 30 | 1,2,3-benzenetriol sulfate (2)_Chemical_Xenobiotics | 4-acetamidophenol_Drug - Analgesics, Anesthetics_Xenobiotics | glucuronide of C10H18O2 (8)*_Partially Characterized Molecules_Partially Characterized Molecules | (S)-a-amino-omega-caprolactam_Food Component/Plant_Xenobiotics |
| 31 | 2-methoxyacetaminophen sulfate*_Drug - Analgesics, Anesthetics_Xenobiotics | N6-methyladenosine_Purine Metabolism, Adenine containing_Nucleotide | 4-hydroxycoumarin_Drug - Cardiovascular_Xenobiotics | X - 24952_NA_NA |
| 32 | X - 12407_NA_NA | N-acetylvaline_Leucine, Isoleucine and Valine Metabolism_Amino Acid | caprylate (8:0)_Medium Chain Fatty Acid_Lipid | X - 12117_NA_NA |
| 33 | docosahexaenoate (DHA; 22:6n3)_Long Chain Polyunsaturated Fatty Acid (n3 and n6)_Lipid | 4-methylguaiaicol sulfate_Benzoate Metabolism_Xenobiotics | X - 12740_NA_NA | vanillic alcohol sulfate_Tyrosine Metabolism_Amino Acid |
| 34 | X - 17690_NA_NA | 2-methoxyacetaminophen glucuronide*_Drug - Analgesics, Anesthetics_Xenobiotics | N-acetylmethionine_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid | X - 24972_NA_NA |

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|----|--|---|---|--|
| 35 | salicylate_Drug - Topical Agents_Xenobiotics | X - 17348_NA_NA | X - 21821_NA_NA | isoursodeoxycholate_Secondary Bile Acid Metabolism_Lipid |
| 36 | X - 17655_NA_NA | X - 24565_NA_NA | sphingomyelin (d18:0/20:0, d16:0/22:0)*_Dihydrosphingomyelins_Lipid | X - 07765_NA_NA |
| 37 | orotidine_Pyrimidine Metabolism, Orotate containing_Nucleotide | 3-(methylthio)acetaminophen sulfate*_Drug - Analgesics, Anesthetics_Xenobiotics | 1-methylhistidine_Histidine Metabolism_Amino Acid | sphingomyelin (d18:2/23:1)*_Sphingomyelins_Lipid |
| 38 | 3-phosphoglycerate_Glycolysis, Gluconeogenesis, and Pyruvate Metabolism_Carbohydrate | beta-citrylglutamate_Glutamate Metabolism_Amino Acid | X - 21815_NA_NA | N-delta-acetylornithine_Urea cycle; Arginine and Proline Metabolism_Amino Acid |
| 39 | sulfate of piperine metabolite C16H19NO3 (2)*_Food Component/Plant_Xenobiotics | sulfate of piperine metabolite C16H19NO3 (3)*_Food Component/Plant_Xenobiotics | DSGEGDFXAEAGGGVR*_Fibrinogen Cleavage Peptide_Peptide | 4-acetaminophen sulfate_Drug - Analgesics, Anesthetics_Xenobiotics |
| 40 | X - 12818_NA_NA | cystine_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid | X - 11483_NA_NA | X - 12730_NA_NA |
| 41 | maltol sulfate_Food Component/Plant_Xenobiotics | X - 15674_NA_NA | X - 11852_NA_NA | saccharin_Food Component/Plant_Xenobiotics |
| 42 | X - 12847_NA_NA | 2-hydroxyoctanoate_Fatty Acid, Monohydroxy_Lipid | (R)-3-hydroxybutyrylcarnitine_Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)_Lipid | X - 11847_NA_NA |
| 43 | N-acetylisoleucine_Leucine, Isoleucine and Valine Metabolism_Amino Acid | lidocaine_Drug - Analgesics, Anesthetics_Xenobiotics | 1-linolenoylglycerol (18:3)_Monoacylglycerol_Lipid | 5-acetylamino-6-formylamino-3-methyluracil_Xanthine Metabolism_Xenobiotics |
| 44 | uracil_Pyrimidine Metabolism, Uracil containing_Nucleotide | androstenediol (3beta,17beta) monosulfate (1)_Androgenic Steroids_Lipid | erucate (22:1n9)_Long Chain Monounsaturated Fatty Acid_Lipid | 5-dodecenoate (12:1n7)_Medium Chain Fatty Acid_Lipid |
| 45 | glycolithocholate_Secondary Bile Acid Metabolism_Lipid | arachidonoylcholine_Fatty Acid Metabolism (Acyl Choline)_Lipid | oleoylcholine_Fatty Acid Metabolism (Acyl Choline)_Lipid | biliverdin_Hemoglobin and Porphyrin Metabolism_Cofactors and Vitamins |
| 46 | X - 12127_NA_NA | 3-hydroxy-2-methylpyridine sulfate_Chemical_Xenobiotics | X - 17328_NA_NA | stearidonate (18:4n3)_Long Chain Polyunsaturated Fatty Acid (n3 and n6)_Lipid |
| 47 | androstenediol (3beta,17beta) monosulfate (2)_Androgenic Steroids_Lipid | sucrose_Disaccharides and Oligosaccharides_Carbohydrate | X - 16946_NA_NA | cystathionine_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid |
| 48 | 1-myristoylglycerol (14:0)_Monoacylglycerol_Lipid | N6-carboxymethyllysine_Advanced Glycation End-product_Carbohydrate | pipecolate_Lysine Metabolism_Amino Acid | pyridoxate_Vitamin B6 Metabolism_Cofactors and Vitamins |
| 49 | methyl-4-hydroxybenzoate sulfate_Benzoate Metabolism_Xenobiotics | X - 23644_NA_NA | S-methylmethionine_Methionine, Cysteine, SAM and Taurine Metabolism_Amino Acid | tauro-beta-muricholate_Primary Bile Acid Metabolism_Lipid |
| 50 | laurate (12:0)_Medium Chain Fatty Acid_Lipid | taurodeoxycholate_Secondary Bile Acid Metabolism_Lipid | X - 16576_NA_NA | butyrylcarnitine (C4)_Fatty Acid Metabolism (also BCAA Metabolism)_Lipid |

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| 51 | 5alpha-androstan-3beta,17beta-diol disulfate_Androgenic Steroids_Lipid | inosine_Purine Metabolism, (Hypo)Xanthine/Inosine containing_Nucleotide | 4-allylcatechol sulfate_Benzoate Metabolism_Xenobiotics | X - 16124_NA_NA |
|----|--|---|---|-----------------|

Table S3. Metabolites chosen in each of the final machine learning models.

| | lgbm (Light GBM) | lg (Logistic regression) | rf (Random forests) |
|----|--|---|--|
| 0 | X_11308_NA_NA | X_24970_NA_NA | X_11308_NA_NA |
| 1 | X_24970_NA_NA | X_11372_NA_NA | perfluorooctanoate_PFOA_Chemical_Xenobiotics |
| 2 | perfluorooctanoate_PFOA_Chemical_Xenobiotics | X_11308_NA_NA | N_acetyl_2_aminooctanoate_Fatty Acid_Amino_Lipid |
| 3 | X_24307_NA_NA | X_14939_NA_NA | X_24970_NA_NA |
| 4 | X_11372_NA_NA | fructose_Fructose_Mannose and Galactose Metabolism_Carbohydrate | N6_methyllysine_Lysine Metabolism_Amino Acid |
| 5 | X_17653_NA_NA | 1_1_etyl_palmitoyl_GPC_P_16_0_Lysoplasmalogen_Lipid | X_23636_NA_NA |
| 6 | X_12112_NA_NA | ferulic acid 4_sulfate_Food Component_Plant_Xenobiotics | methionine sulfone_Methionine_Cysteine_SAM and Taurine Metabolism_Amino Acid |
| 7 | | ribulonate_xylulonate_lyxonate_Pentose Metabolism_Carbohydrate | |
| 8 | | X_17676_NA_NA | |
| 9 | | X_12680_NA_NA | |
| 10 | | 4_vinylguaiacol sulfate_Food Component_Plant_Xenobiotics | |
| 11 | | X_11444_NA_NA | |
| 12 | | X_24432_NA_NA | |
| 13 | | 3_hydroxystachydrine_Food Component_Plant_Xenobiotics | |
| 14 | | 1_palmitoyl_2_palmitoleoyl_GPC_P_16_0_16_1_Phosphatidylcholine_PC_Lipid | |
| 15 | | ethyl alpha_glucopyranoside_Food Component_Plant_Xenobiotics | |
| 16 | | 1_2_dilinoleoyl_GPC_P_18_2_18_2_Phosphatidylcholine_PC_Lipid | |
| 17 | | metabolonic lactone sulfate_Partially Characterized Molecules_Partially Characterized Molecules | |
| 18 | | X_24337_NA_NA | |
| 19 | | X_21353_NA_NA | |
| 20 | | behenoyl sphingomyelin_d18_1_22_0_Sphingomyelins_Lipid | |
| 21 | | 1_1_etyl_palmitoyl_2_linoleoyl_GPC_P_16_0_18_2_Plasmalogen_Lipid | |
| 22 | | sphingomyelin_d18_1_22_1_d18_2_22_0_d16_1_24_1_Sphingomyelins_Lipid | |
| 23 | | N_methylpipecolate_Bacterial_Fungal_Xenobiotics | |
| 24 | | 1_lignoceroyl_GPC_P_24_0_Lysophospholipid_Lipid | |
| 25 | | X_21448_NA_NA | |

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| 2 6 | | branched_chain_straight_chain_or cyclopropyl 10_1 fatty acid_1__Partially Characterized Molecules_Partially Characterized Molecules | |
| 2 7 | | 1_1_enyl_palmitoyl_2_palmitoyl_GPC P_16_0_16_0__Plasmalogen_Lipid | |
| 2 8 | | X_12524_NA_NA | |
| 2 9 | | octadecenedioylcarnitine_C18_1_DC__Fatty Acid Metabolism_Acyl Carnitine_Dicarboxylate__Lipid | |
| 3 0 | | 1_stearoyl_2_oleoyl_GPI 18_0_18_1__Phosphatidylinositol_PI__Lipid | |
| 3 1 | | creatinine_Creatine Metabolism_Amino Acid | |
| 3 2 | | sphingomyelin_d18_1_21_0_d17_1_22_0_ d16_1_23_0__Sphingomyelins_Lipid | |
| 3 3 | | X_12112_NA_NA | |
| 3 4 | | X_13728_NA_NA | |
| 3 5 | | X_23636_NA_NA | |
| 3 6 | | X_21410_NA_NA | |
| 3 7 | | 4_methoxyphenol sulfate_Tyrosine Metabolism_Amino Acid | |
| 3 8 | | X_18922_NA_NA | |
| 3 9 | | X_16397_NA_NA | |
| 4 0 | | alpha_ketobutyrate_Methionine_Cysteine_SAM and Taurine Metabolism_Amino Acid | |
| 4 1 | | hypotaurine_Methionine_Cysteine_SAM and Taurine Metabolism_Amino Acid | |
| 4 2 | | 2_hydroxybutyrate_2_hydroxyisobutyrate_Glutathion e Metabolism_Amino Acid | |
| 4 3 | | 3_methylglutaconate_Leucine_Isoleucine and Valine Metabolism_Amino Acid | |
| 4 4 | | glucuronide of C12H22O4_1__Partially Characterized Molecules_Partially Characterized Molecules | |
| 4 5 | | octadecenedioate_C18_1_DC__Fatty Acid_ Dicarboxylate_Lipid | |
| 4 6 | | octadecadienedioate_C18_2_DC__Fatty Acid_ Dicarboxylate_Lipid | |
| 4 7 | | 1_stearoyl_2_linoleoyl_GPC 18_0_18_2__Phosphatidylcholine_PC__Lipid | |
| 4 8 | | myristoleoylcarnitine_C14_1__Fatty Acid Metabolism_Acyl Carnitine_ Monounsaturated_Lipid | |
| 4 9 | | X_14056_NA_NA | |
| 5 0 | | X_12729_NA_NA | |
| 5 1 | | 1_oleoyl_GPC_18_1__Lysophospholipid_Lipid | |
| 5 2 | | 1_ribosyl_imidazoleacetate__Histidine Metabolism_Amino Acid | |
| 5 3 | | 1_dihomo_linolenylglycerol 20_3__Monoacylglycerol_Lipid | |
| 5 4 | | cysteinylglycine disulfide__Glutathione Metabolism_Amino Acid | |
| 5 5 | | X_12100_NA_NA | |

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|--------|--|--|--|
| 5 6 | | arabonate_xylonate_Pentose Metabolism_Carbohydrate | |
| 5 7 | | glycine_Glycine_Serine and Threonine Metabolism_Amino Acid | |
| 5 8 | | 1_1_etyl_palmitoyl_2_palmitoleoyl_GPC P_16_0_16_1_Plasmalogen_Lipid | |
| 5 9 | | X_21383_NA_NA | |
| 6 0 | | glycerophosphoglycerol_Glycerolipid Metabolism_Lipid | |
| 6 1 | | 1_palmitoleoylglycerol 16_1_Monoacylglycerol_Lipid | |
| 6 2 | | N1_methylinosine_Purine Metabolism_ Hypo_Xanthine_Inosine containing_Nucleotide | |
| 6 3 | | X_11880_NA_NA | |
| 6 4 | | X_11470_NA_NA | |
| 6 5 | | X_21319_NA_NA | |
| 6 6 | | X_24947_NA_NA | |
| 6 7 | | X_12906_NA_NA | |
| 6 8 | | sphingomyelin_d18_1_17_0_d17_1_18_0_ d19_1_16_0_Sphingomyelins_Lipid | |
| 6 9 | | X_12104_NA_NA | |
| 7 0 | | 1_1_etyl_stearoyl_2_oleoyl_GPE P_18_0_18_1_Plasmalogen_Lipid | |
| 7 1 | | X_23665_NA_NA | |
| 7 2 | | X_22162_NA_NA | |
| 7 3 | | X_13553_NA_NA | |
| 7 4 | | heptenedioate_C7_1_DC_Fatty Acid_ Dicarboxylate_Lipid | |

Table S4. Metabolites chosen in each of the final machine learning models without xenobiotics.

| | lgbm (Light GBM) | lg (Logistic regression) | rf (Random forests) |
|----|--|--|---|
| 0 | X_11308_NA_NA | X_11308_NA_NA | X_11308_NA_NA |
| 1 | X_24970_NA_NA | X_11372_NA_NA | 3_carboxy_4_methyl_5_propyl_2_furanpropanoate_CMPF_Fatty Acid_Dicarboxylate_Lipid |
| 2 | X_24307_NA_NA | X_24970_NA_NA | X_24970_NA_NA |
| 3 | gulonate_Ascorbate and Aldarate Metabolism_Cofactors and Vitamins | X_16935_NA_NA | N6_N6_dimethyllysine_Lysine Metabolism_Amino Acid |
| 4 | N_acetyltaurine_Methionine_Cysteine_SAM and Taurine Metabolism_Amino Acid | X_11880_NA_NA | bilirubin_Hemoglobin and Porphyrin Metabolism_Cofactors and Vitamins |
| 5 | fructose_Fructose_Mannose and Galactose Metabolism_Carbohydrate | N6_methyllysine_Lysine Metabolism_Amino Acid | sphingomyelin_d18_1_20_1_d18_2_20_0_Sphingomyelins_Lipid |
| 6 | arabonate_xylonate_Pentose Metabolism_Carbohydrate | phenylpyruvate_Phenylalanine Metabolism_Amino Acid | 5_methyluridine_ribothymidine_Pyrimidine Metabolism_Uracil containing_Nucleotide |
| 7 | 1_oleoyl_GPC_18_1_Lysophospholipid_Lipid | gamma_glutamyl_epsilon_lysine_Gamma_glutamyl_Amino Acid_Peptide | |
| 8 | X_13431_NA_NA | hydroxy_CMPF_Fatty Acid_Dicarboxylate_Lipid | |
| 9 | X_12112_NA_NA | behenoyl sphingomyelin_d18_1_22_0_Sphingomyelins_Lipid | |
| 10 | X_12100_NA_NA | 2_palmitoyl_GPC_16_0_Lysophospholipid_Lipid | |
| 11 | X_18921_NA_NA | X_23666_NA_NA | |
| 12 | X_12104_NA_NA | N6_N6_dimethyllysine_Lysine Metabolism_Amino Acid | |
| 13 | X_17676_NA_NA | sphingomyelin_d18_1_22_1_d18_2_22_0_d16_1_24_1_Sphingomyelins_Lipid | |
| 14 | mannose_Fructose_Mannose and Galactose Metabolism_Carbohydrate | X_11441_NA_NA | |
| 15 | X_15503_NA_NA | methionine sulfone_Methionine_Cysteine_SAM and Taurine Metabolism_Amino Acid | |
| 16 | X_12193_NA_NA | X_15245_NA_NA | |
| 17 | X_21829_NA_NA | retinol_Vitamin A_Vitamin A Metabolism_Cofactors and Vitamins | |
| 18 | 2_palmitoleoyl_GPC_16_1_Lysophospholipid_Lipid | 1_linoleoyl_GPG_18_2_Lysophospholipid_Lipid | |
| 19 | 9_hydroxystearate_Fatty Acid_Monohydroxy_Lipid | X_15503_NA_NA | |
| 20 | sphingomyelin_d18_1_24_1_d18_2_24_0_Sphingomyelins_Lipid | glutamate_Glutamate Metabolism_Amino Acid | |
| 21 | sphingomyelin_d18_2_14_0_d18_1_14_1_Sphingomyelins_Lipid | dehydroepiandrosterone sulfate_DHEA_S_Androgenic Steroids_Lipid | |
| 22 | X_18887_NA_NA | 4_hydroxyglutamate_Glutamate Metabolism_Amino Acid | |
| 23 | X_22162_NA_NA | androstenediol_3alpha_17alpha_monosulfate_3_Androgenic Steroids_Lipid | |
| 24 | X_12680_NA_NA | X_12524_NA_NA | |
| 25 | X_12101_NA_NA | X_21364_NA_NA | |
| 26 | myristoleoylcarnitine_C14_1_Fatty Acid Metabolism_Acyl Carnitine_Monounsaturated_Lipid | 3_amino_2_piperidone_Urea cycle_Arginine and Proline Metabolism_Amino Acid | |

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|----|---|--|--|
| 27 | X_22771_NA_NA | andro steroid monosulfate C19H28O6S_1___Androgenic Steroids_Lipid | |
| 28 | 1_1_1_enyl_palmitoyl_2_palmitoyl_GPC P_16_0_16_0___Plasmalogen_Lipid | taurochenodeoxycholic acid 3_sulfate_Secondary Bile Acid Metabolism_Lipid | |
| 29 | X_19141_NA_NA | sphingomyelin_d18_1_20_0_ d16_1_22_0___Sphingomyelins_Lipid | |
| 30 | X_21467_NA_NA | 3_4_hydroxyphenyl_lactate _HPLA___Tyrosine Metabolism_Amino Acid | |
| 31 | X_21470_NA_NA | tricosanoyl sphingomyelin _d18_1_23_0___Sphingomyelins_Lipi d | |
| 32 | X_21471_NA_NA | isovalerate_C5___Leucine_Isoleucine and Valine Metabolism_Amino Acid | |
| 33 | alpha_hydroxyisovalerate_Leucine_ Isoleucine and Valine Metabolism_Amino Acid | sphingomyelin_d18_2_23_0_ d18_1_23_1_ d17_1_24_1___Sphingomyelins_Lipid | |
| 34 | N_acetylglucosamine_N_acetylgalactosami ne_Aminosugar Metabolism_Carbohydrate | dihomo_linoleoylcarnitine _C20_2___Fatty Acid Metabolism _Acyl Carnitine_ Polyunsaturated___Lipid | |
| 35 | 3_methylglutaryl carnitine_2___Leucine_ Isoleucine and Valine Metabolism_Amino Acid | X_14939_NA_NA | |
| 36 | X_11299_NA_NA | sphingomyelin_d17_2_16_0_ d18_2_15_0___Sphingomyelins_Lipid | |
| 37 | X_11372_NA_NA | tetradecanedioate_C14___Fatty Acid_ Dicarboxylate_Lipid | |
| 38 | X_11470_NA_NA | N2_N2_dimethylguanosine_Purine Metabolism_Guanine containing_Nucleotide | |
| 39 | X_11478_NA_NA | 1_linoleoyl_2_arachidonoyl_GPC _18_2_20_4n6___Phosphatidylcholin e_PC___Lipid | |
| 40 | X_17654_NA_NA | 1_palmitoyl_2_oleoyl_GPC _16_0_18_1___Phosphatidylcholine PC___Lipid | |
| 41 | X_21736_NA_NA | 1_1_enyl_palmitoyl_2_oleoyl_GPE P_16_0_18_1___Plasmalogen_Lipid | |
| 42 | 1_dihomo_linolenylglycerol _20_3___Monoacylglycerol_Lipid | ceramide_d18_1_14_0_ d16_1_16_0___Ceramides_Lipid | |
| 43 | X_17351_NA_NA | X_23997_NA_NA | |
| 44 | X_16397_NA_NA | 1_1_enyl_palmitoyl_GPC P_16_0___Lysoplasmalogen_Lipid | |
| 45 | X_16580_NA_NA | 2_oleoylglycerol _18_1___Monoacylglycerol_Lipid | |
| 46 | bilirubin_E_Z or Z_E___Hemoglobin and Porphyrin Metabolism_Cofactors and Vitamins | guanidinoacetate_Creatine Metabolism_Amino Acid | |
| 47 | X_12026_NA_NA | N1_methylinosine_Purine Metabolism_ _Hypo_Xanthine_Inosine containing_Nucleotide | |
| 48 | X_12221_NA_NA | 2_hydroxy_3_methylvalerate_Leucine _Isoleucine and Valine Metabolism_Amino Acid | |
| 49 | X_12906_NA_NA | X_21448_NA_NA | |
| 50 | X_13553_NA_NA | 4_hydroxy_2_oxoglutaric acid_Fatty Acid_Dicarboxylate_Lipid | |

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|----|--|---|--|
| 51 | X_17357_NA_NA | 3_methoxytyrosine_Tyrosine Metabolism_Amino Acid | |
| 52 | X_18899_NA_NA | urate_Purine Metabolism_Hypo_Xanthine_Inosine containing_Nucleotide | |
| 53 | 1_1_enyl_stearoyl_2_linoleoyl_GPE_P_18_0_18_2__Plasmalogen_Lipid | sphingomyelin_d18_0_18_0_d19_0_17_0__Dihydrosphingomyelins_Lipid | |
| 54 | X_21448_NA_NA | palmitoyl sphingomyelin_d18_1_16_0__Sphingomyelins_Lipid | |
| 55 | cysteinylglycine disulfide__Glutathione Metabolism_Amino Acid | tiglyl carnitine_C5__Leucine_Isoleucine and Valine Metabolism_Amino Acid | |
| 56 | X_24947_NA_NA | 1_arachidonoyl_GPI_20_4__Lysophospholipid_Lipid | |
| 57 | X_24951_NA_NA | 1_1_enyl_stearoyl_2_linoleoyl_GPE_P_18_0_18_2__Plasmalogen_Lipid | |
| 58 | uridine_Pyrimidine Metabolism_Uracil containing_Nucleotide | 5_hydroxylysine_Lysine Metabolism_Amino Acid | |
| 59 | nisinate_24_6n3__Long Chain Polyunsaturated Fatty Acid_n3 and n6__Lipid | N_acetylneuraminate_Aminosugar Metabolism_Carbohydrate | |
| 60 | N_1__N_8__acetylspermidine_Polyamine Metabolism_Amino Acid | isoleucine_Leucine_Isoleucine and Valine Metabolism_Amino Acid | |
| 61 | glycine_Glycine_Serine and Threonine Metabolism_Amino Acid | X_21471_NA_NA | |
| 62 | histidine_Histidine Metabolism_Amino Acid | kynurenate_Tryptophan Metabolism_Amino Acid | |
| 63 | hypotaurine_Methionine_Cysteine_SAM and Taurine Metabolism_Amino Acid | X_24947_NA_NA | |
| 64 | leucine_Leucine_Isoleucine and Valine Metabolism_Amino Acid | palmitoyl_sphingosine_phosphoethanolamine_d18_1_16_0__Ceramide PEs_Lipid | |
| 65 | dihydroorotate_Pyrimidine Metabolism_Orotate containing_Nucleotide | linoleoylcarnitine_C18_2__Fatty Acid Metabolism_Acyl Carnitine_Polyunsaturated__Lipid | |
| 66 | gamma_glutamylcitrulline__Gamma_glutamyl Amino Acid_Peptide | sphingomyelin_d18_2_24_2__Sphingomyelins_Lipid | |
| 67 | N_oleoylserine_Endocannabinoid_Lipid | N_oleoylserine_Endocannabinoid_Lipid | |
| 68 | glycine conjugate of C10H14O2_1__Partially Characterized Molecules_Partially Characterized Molecules | 1_linolenoyl_GPC_18_3__Lysophospholipid_Lipid | |