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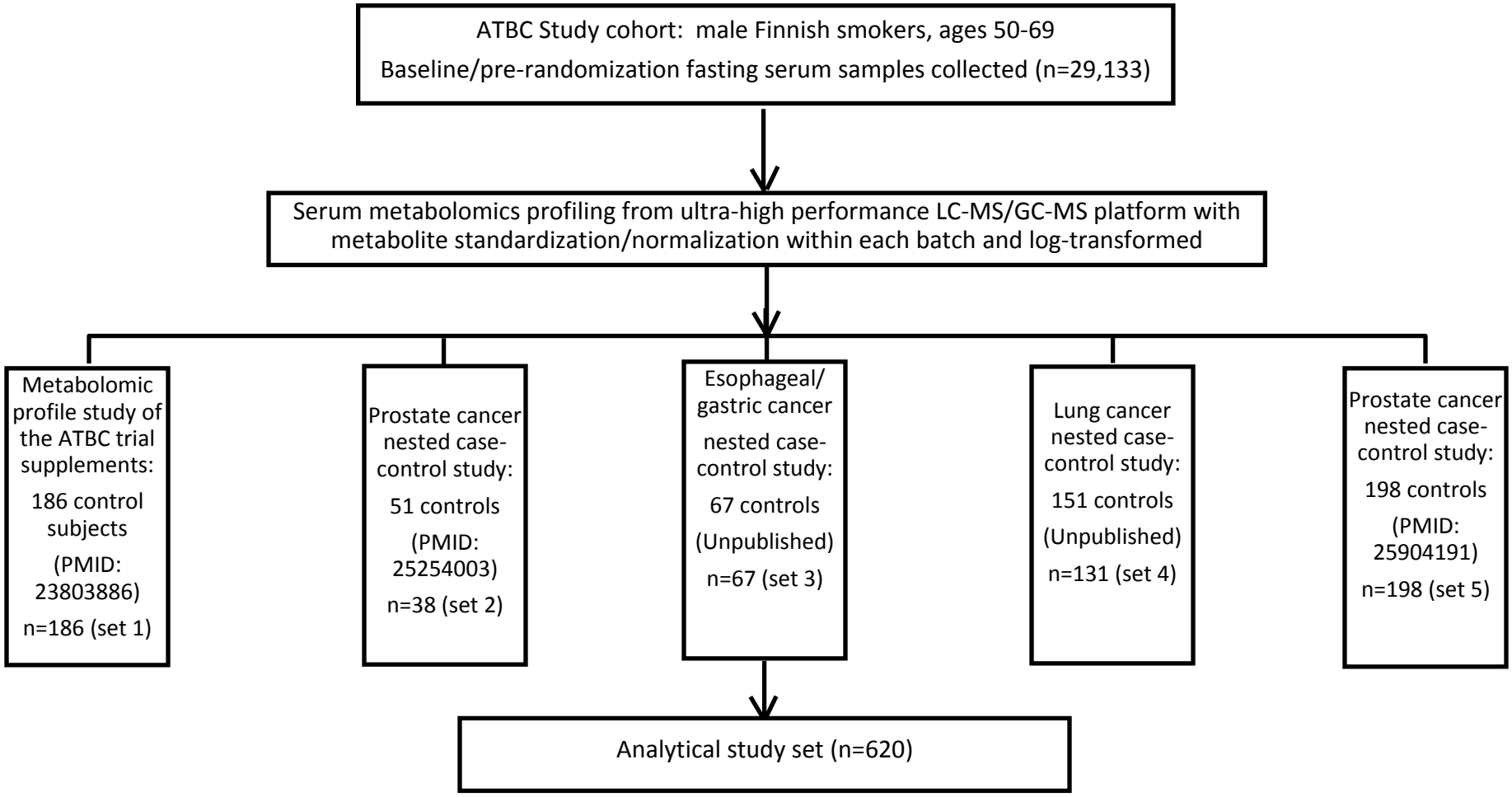
Web Figure 1. Participant Flow Chart for Associations Between the Serum Metabolomic Profiling and All-Cause Mortality: A Prospective Analysis in the Alpha-Tocopherol, Beta-Carotene Cancer Prevention (ATBC) Study (1985-2013). [a]



[a] Sample sizes may differ from the original study sets because of some duplicate participants across the studies. The two sets of prostate cancer study controls are different individuals. The present analysis is based on non-cancer, control participants previously selected for one of five metabolomic studies nested within the ATBC Study (control participants: they are cancer-free individuals at the index date, but they were able to develop cancer during the follow-up period).

Web Table 1. List of Measured Known Metabolites in the ATBC Study (1985-2013).

Metabolite	Reported in the present study	Super pathway	Sub pathway
Alanine	Yes	Amino acid	Alanine and aspartate metabolism
Asparagine	Yes	Amino acid	Alanine and aspartate metabolism
Aspartate	Yes	Amino acid	Alanine and aspartate metabolism
N_acetylalanine	Yes	Amino acid	Alanine and aspartate metabolism
_2_aminobutyrate	Yes	Amino acid	Butanoate metabolism; cysteine, methionine, sam, taurine metabolism
Creatine	Yes	Amino acid	Creatine metabolism
Creatinine	Yes	Amino acid	Creatine metabolism
_2_hydroxybutyrate__ahb_	Yes	Amino acid	Cysteine, methionine, SAM, taurine metabolism
Cysteine	Yes	Amino acid	Cysteine, methionine, SAM, taurine metabolism
Cystine	Yes	Amino acid	Cysteine, methionine, SAM, taurine metabolism
Methionine	Yes	Amino acid	Cysteine, methionine, SAM, taurine metabolism
N_acetylmethionine	Yes	Amino acid	Cysteine, methionine, SAM, taurine metabolism
N_formylmethionine	Yes	Amino acid	Cysteine, methionine, SAM, taurine metabolism
S_methylcysteine	Yes	Amino acid	Cysteine, methionine, SAM, taurine metabolism
Taurine	Yes	Amino acid	Cysteine, methionine, SAM, taurine metabolism
Glutamate	Yes	Amino acid	Glutamate metabolism
Glutamine	Yes	Amino acid	Glutamate metabolism
Pyroglutamine	Yes	Amino acid	Glutamate metabolism
_5_oxoproline	Yes	Amino acid	Glutathione metabolism
Cysteine_glutathione_disulfid	Yes	Amino acid	Glutathione metabolism
Betaine	Yes	Amino acid	Glycine, serine and threonine metabolism
Dimethylglycine	Yes	Amino acid	Glycine, serine and threonine metabolism
Glycine	Yes	Amino acid	Glycine, serine and threonine metabolism
N_acetylglycine	Yes	Amino acid	Glycine, serine and threonine metabolism
N_acetylserine	Yes	Amino acid	Glycine, serine and threonine metabolism
N_acetylthreonine	Yes	Amino acid	Glycine, serine and threonine metabolism
Serine	Yes	Amino acid	Glycine, serine and threonine metabolism
Threonine	Yes	Amino acid	Glycine, serine and threonine

			metabolism
_4_guanidinobutanoate	Yes	Amino acid	Guanidino and acetamido metabolism
_4_acetamidobutanoate	Yes	Amino acid	Guanidino and acetamido metabolism; polyamine metabolism
_1_methylhistidine	Yes	Amino acid	Histidine metabolism
_1_methylimidazoleacetate	Yes	Amino acid	Histidine metabolism
_3_methylhistidine	Yes	Amino acid	Histidine metabolism
Histidine	Yes	Amino acid	Histidine metabolism
Imidazole_propionate	Yes	Amino acid	Histidine metabolism
Trans_urocanate	Yes	Amino acid	Histidine metabolism
_2_aminoadipate	Yes	Amino acid	Lysine metabolism
Glutarylcarnitine	Yes	Amino acid	Lysine metabolism
Lysine	Yes	Amino acid	Lysine metabolism
N6_acetyllysine	Yes	Amino acid	Lysine metabolism
Pipecolate	Yes	Amino acid	Lysine metabolism
_3__3_hydroxyphenyl_propionat	Yes	Amino acid	Phenylalanine & tyrosine metabolism
_3__4_hydroxyphenyl_lactate	Yes	Amino acid	Phenylalanine & tyrosine metabolism
_3_methoxytyrosine	Yes	Amino acid	Phenylalanine & tyrosine metabolism
_3_phenylpropionate	Yes	Amino acid	Phenylalanine & tyrosine metabolism
_4_hydroxyphenylpyruvate	Yes	Amino acid	Phenylalanine & tyrosine metabolism
Gentisate	Yes	Amino acid	Phenylalanine & tyrosine metabolism
N_acetylphenylalanine	Yes	Amino acid	Phenylalanine & tyrosine metabolism
N_acetyltyrosine	Yes	Amino acid	Phenylalanine & tyrosine metabolism
O_cresol_sulfate	Yes	Amino acid	Phenylalanine & tyrosine metabolism
P_cresol_sulfate	Yes	Amino acid	Phenylalanine & tyrosine metabolism
Phenol_sulfate	Yes	Amino acid	Phenylalanine & tyrosine metabolism
Phenylacetate	Yes	Amino acid	Phenylalanine & tyrosine metabolism
Phenylacetylglutamine	Yes	Amino acid	Phenylalanine & tyrosine metabolism
Phenylalanine	Yes	Amino acid	Phenylalanine & tyrosine metabolism
Phenyllactate__pla_	Yes	Amino acid	Phenylalanine & tyrosine metabolism
Tyrosine	Yes	Amino acid	Phenylalanine & tyrosine metabolism
_5_methylthioadenosine__mta_	Yes	Amino acid	Polyamine metabolism
Acisoga	Yes	Amino acid	Polyamine metabolism
N_acetylputrescine	Yes	Amino acid	Polyamine metabolism
_3_indoxyl_sulfate	Yes	Amino acid	Tryptophan metabolism
C_glycosyltryptophan	Yes	Amino acid	Tryptophan metabolism
Indoleacetate	Yes	Amino acid	Tryptophan metabolism
Indoleacetylglutamine	Yes	Amino acid	Tryptophan metabolism
Indolelactate	Yes	Amino acid	Tryptophan metabolism
Indolepropionate	Yes	Amino acid	Tryptophan metabolism
Kynurenate	Yes	Amino acid	Tryptophan metabolism
Kynurenine	Yes	Amino acid	Tryptophan metabolism
N_acetyltryptophan	Yes	Amino acid	Tryptophan metabolism

Tryptophan	Yes	Amino acid	Tryptophan metabolism
Tryptophan_betaine	Yes	Amino acid	Tryptophan metabolism
Arginine	Yes	Amino acid	Urea cycle; arginine and proline metabolism
Citrulline	Yes	Amino acid	Urea cycle; arginine and proline metabolism
Dimethylarginine__sdma___adma	Yes	Amino acid	Urea cycle; arginine and proline metabolism
Homocitrulline	Yes	Amino acid	Urea cycle; arginine and proline metabolism
N_delta_acetylornithine	Yes	Amino acid	Urea cycle; arginine and proline metabolism
N_methyl_proline	Yes	Amino acid	Urea cycle; arginine and proline metabolism
Ornithine	Yes	Amino acid	Urea cycle; arginine and proline metabolism
Trans_4_hydroxyproline	Yes	Amino acid	Urea cycle; arginine and proline metabolism
Urea	Yes	Amino acid	Urea cycle; arginine and proline metabolism
_2_hydroxy_3_methylvalerate	Yes	Amino acid	Valine, leucine and isoleucine metabolism
_3_hydroxy_2_ethylpropionate	Yes	Amino acid	Valine, leucine and isoleucine metabolism
_3_hydroxyisobutyrate	Yes	Amino acid	Valine, leucine and isoleucine metabolism
_3_methyl_2_oxobutyrate	Yes	Amino acid	Valine, leucine and isoleucine metabolism
_3_methyl_2_oxovalerate	Yes	Amino acid	Valine, leucine and isoleucine metabolism
_4_methyl_2_oxopentanoate	Yes	Amino acid	Valine, leucine and isoleucine metabolism
Alpha_hydroxyisocaproate	Yes	Amino acid	Valine, leucine and isoleucine metabolism
Alpha_hydroxyisovalerate	Yes	Amino acid	Valine, leucine and isoleucine metabolism
Beta_hydroxyisovalerate	Yes	Amino acid	Valine, leucine and isoleucine metabolism
Isobutyrylcarnitine	Yes	Amino acid	Valine, leucine and isoleucine metabolism
Isoleucine	Yes	Amino acid	Valine, leucine and isoleucine metabolism
Isovalerylcarnitine	Yes	Amino acid	Valine, leucine and isoleucine metabolism
Isovalerylglycine	Yes	Amino acid	Valine, leucine and isoleucine metabolism
Leucine	Yes	Amino acid	Valine, leucine and isoleucine metabolism
N_acetylisoleucine	Yes	Amino acid	Valine, leucine and isoleucine metabolism
N_acetylleucine	Yes	Amino acid	Valine, leucine and isoleucine

			metabolism
N_acetylvaline	Yes	Amino acid	Valine, leucine and isoleucine metabolism
Tiglyl_carnitine	Yes	Amino acid	Valine, leucine and isoleucine metabolism
Valine	Yes	Amino acid	Valine, leucine and isoleucine metabolism
_3_ureidopropionate	Yes	Amino acid; nucleotide	Alanine and aspartate metabolism; pyrimidine metabolism, uracil containing
Beta_alanine	Yes	Amino acid; nucleotide	Alanine and aspartate metabolism; pyrimidine metabolism, uracil containing
N_acetyl_beta_alanine	Yes	Amino acid; nucleotide	Alanine and aspartate metabolism; pyrimidine metabolism, uracil containing
Levulinate__4_oxovalerate_	Yes	Amino aicd; xenobiotics	Valine, leucine and isoleucine metabolism; food component/plant
Erythronate	Yes	Carbohydrate	Aminosugar metabolism
Fucose	Yes	Carbohydrate	Aminosugar metabolism; pentose metabolism
Fructose	Yes	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism
Mannitol	Yes	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism
Mannose	Yes	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism
_1_5_anhydroglucitol__1_5_ag_	Yes	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism
Glucose	Yes	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism
Glycerate	Yes	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism
Lactate	Yes	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism
Pyruvate	Yes	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism
Arabinose	Yes	Carbohydrate	Pentose metabolism
Arabitol	Yes	Carbohydrate	Pentose metabolism
Ribitol	Yes	Carbohydrate	Pentose metabolism
Ribose	Yes	Carbohydrate	Pentose metabolism
Ribulose	Yes	Carbohydrate	Pentose metabolism
Threitol	Yes	Carbohydrate	Pentose metabolism
Xylitol	Yes	Carbohydrate	Pentose metabolism
Xylonate	Yes	Carbohydrate	Pentose metabolism
Xylose	Yes	Carbohydrate	Pentose metabolism
Oxalate__ethanedioate_	Yes	Carbohydrate; cofactors and vitamins	Glyoxylate and dicarboxylate metabolism; ascorbate and aldarate metabolism

_1_6_anhydroglucose	Yes	Carbohydrate; xenobiotics	Glycolysis, gluconeogenesis, pyruvate metabolism; food component/plant
Gluconate	Yes	Carbohydrate; xenobiotics	Pentose metabolism; food component/plant
Arabonate	Yes	Cofactors and vitamins	Ascorbate and aldarate metabolism
Ascorbate__vitamin_c_	Yes	Cofactors and vitamins	Ascorbate and aldarate metabolism
Threonate	Yes	Cofactors and vitamins	Ascorbate and aldarate metabolism
Bilirubin__e_e_	Yes	Cofactors and vitamins	Hemoglobin and porphyrin metabolism
Bilirubin__z_z_	Yes	Cofactors and vitamins	Hemoglobin and porphyrin metabolism
Biliverdin	Yes	Cofactors and vitamins	Hemoglobin and porphyrin metabolism
Heme	Yes	Cofactors and vitamins	Hemoglobin and porphyrin metabolism
L_urobilin	Yes	Cofactors and vitamins	Hemoglobin and porphyrin metabolism
N1_methyl_2_pyridone_5_carbox	Yes	Cofactors and vitamins	Nicotinate and nicotinamide metabolism
Nicotinamide	Yes	Cofactors and vitamins	Nicotinate and nicotinamide metabolism
Trigonelline__n__methylnicoti	Yes	Cofactors and vitamins	Nicotinate and nicotinamide metabolism
Pantothenate	Yes	Cofactors and vitamins	Pantothenate and coa metabolism
Riboflavin__vitamin_b2_	Yes	Cofactors and vitamins	Riboflavin metabolism
Alpha_tocopherol	Yes	Cofactors and vitamins	Tocopherol metabolism
Beta_tocopherol	Yes	Cofactors and vitamins	Tocopherol metabolism
Gamma_cehc	Yes	Cofactors and vitamins	Tocopherol metabolism
Gamma_cehc_glucuronide	Yes	Cofactors and vitamins	Tocopherol metabolism
Gamma_tocopherol	Yes	Cofactors and vitamins	Tocopherol metabolism
Pyridoxate	Yes	Cofactors and vitamins	Vitamin b6 metabolism; pyridoxal metabolism
Alpha_ketoglutarate	Yes	Energy	Krebs cycle / tca cycle
Citrate	Yes	Energy	Krebs cycle / tca cycle
Fumarate	Yes	Energy	Krebs cycle / tca cycle
Malate	Yes	Energy	Krebs cycle / tca cycle
Succinate	Yes	Energy	Krebs cycle / tca cycle
Succinylcarnitine	Yes	Energy	Krebs cycle / tca cycle
Phosphate	Yes	Energy	Oxidative phosphorylation
_15_methylpalmitate__isobar_w	Yes	Lipid	

Acetylcarnitine	Yes	Lipid	Carnitine metabolism
Carnitine	Yes	Lipid	Carnitine metabolism
Cis_4_decenoyl_carnitine	Yes	Lipid	Carnitine metabolism
Decanoylcarnitine	Yes	Lipid	Carnitine metabolism
Deoxycarnitine	Yes	Lipid	Carnitine metabolism
Hexanoylcarnitine	Yes	Lipid	Carnitine metabolism
Laurylcarnitine	Yes	Lipid	Carnitine metabolism
Myristoylcarnitine	Yes	Lipid	Carnitine metabolism
Octanoylcarnitine	Yes	Lipid	Carnitine metabolism
Oleoylcarnitine	Yes	Lipid	Carnitine metabolism
Palmitoylcarnitine	Yes	Lipid	Carnitine metabolism
Stearoylcarnitine	Yes	Lipid	Carnitine metabolism
_1_2_dipalmitoylglycerol	Yes	Lipid	Diacylglycerol
_1_3_dipalmitoylglycerol	Yes	Lipid	Diacylglycerol
_12_hete	Yes	Lipid	Eicosanoid
Oleic_ethanolamide	Yes	Lipid	Endocannabinoid
Palmitoyl_ethanolamide	Yes	Lipid	Endocannabinoid
Dihomo_linolenate	Yes	Lipid	Essential fatty acid; polyunsaturated fatty acid (n3 and n6)
Docosahexaenoate	Yes	Lipid	Essential fatty acid; polyunsaturated fatty acid (n3 and n6)
Docosapentaenoat	Yes	Lipid	Essential fatty acid; polyunsaturated fatty acid (n3 and n6)
Docosapentaenoate	Yes	Lipid	Essential fatty acid; polyunsaturated fatty acid (n3 and n6)
Eicosapentaenoate	Yes	Lipid	Essential fatty acid; polyunsaturated fatty acid (n3 and n6)
Linoleate__18_2n6_	Yes	Lipid	Essential fatty acid; polyunsaturated fatty acid (n3 and n6)
Linolenate_alpha_or_gamma	Yes	Lipid	Essential fatty acid; polyunsaturated fatty acid (n3 and n6)
Butyrylcarnitine	Yes	Lipid	Fatty acid metabolism (also BCAA metabolism)
Hydroxybutyrylcarnitine	Yes	Lipid	Fatty acid metabolism (also BCAA metabolism)
Propionylcarnitine	Yes	Lipid	Fatty acid metabolism (also BCAA metabolism)
Valerylcarnitine	Yes	Lipid	Fatty acid metabolism; carnitine metabolism
_2_aminooctanoate	Yes	Lipid	Fatty acid, amino
_17_methylstearate	Yes	Lipid	Fatty acid, branched
_2_hydroxyglutarate	Yes	Lipid	Fatty acid, dicarboxylate
Azelate__nonanedioate_	Yes	Lipid	Fatty acid, dicarboxylate
Cmpf	Yes	Lipid	Fatty acid, dicarboxylate
Dodecanedioate	Yes	Lipid	Fatty acid, dicarboxylate
Hexadecanedioate	Yes	Lipid	Fatty acid, dicarboxylate
Octadecanedioate	Yes	Lipid	Fatty acid, dicarboxylate

Sebacate__decanedioate_	Yes	Lipid	Fatty acid, dicarboxylate
Tetradecanedioate	Yes	Lipid	Fatty acid, dicarboxylate
Undecanedioate	Yes	Lipid	Fatty acid, dicarboxylate
_13_hode___9_hode	Yes	Lipid	Fatty acid, monohydroxy
_2_hydroxyoctanoate	Yes	Lipid	Fatty acid, monohydroxy
_2_hydroxypalmitate	Yes	Lipid	Fatty acid, monohydroxy
_2_hydroxystearate	Yes	Lipid	Fatty acid, monohydroxy
_3_hydroxydecanoate	Yes	Lipid	Fatty acid, monohydroxy
_3_hydroxyoctanoate	Yes	Lipid	Fatty acid, monohydroxy
_3_hydroxypropanoate	Yes	Lipid	Fatty acid, monohydroxy
Glycerol	Yes	Lipid	Glycerolipid metabolism
Glycerol_3_phosphate__g3p_	Yes	Lipid	Glycerolipid metabolism
Choline	Yes	Lipid	Glycerolipid metabolism; phospholipid metabolism
Glycerophosphorylcholine__gpc	Yes	Lipid	Glycerolipid metabolism; phospholipid metabolism
Trimethylamine_n_oxide	Yes	Lipid	Glycerolipid metabolism; phospholipid metabolism
Chiro_inositol	Yes	Lipid	Inositol metabolism
Inositol_1_phosphate__i1p_	Yes	Lipid	Inositol metabolism
Myo_inositol	Yes	Lipid	Inositol metabolism
_3_hydroxybutyrate__bhba_	Yes	Lipid	Ketone bodies
Acetoacetate	Yes	Lipid	Ketone bodies
_10_heptadecenoate__17_1n7_	Yes	Lipid	Long chain fatty acid
_10_nonadecenoate__19_1n9_	Yes	Lipid	Long chain fatty acid
Eicosenoate__20_1n9_or_11_	Yes	Lipid	Long chain fatty acid
Margarate__17_0_	Yes	Lipid	Long chain fatty acid
Myristate__14_0_	Yes	Lipid	Long chain fatty acid
Myristoleate__14_1n5_	Yes	Lipid	Long chain fatty acid
Nonadecanoate__19_0_	Yes	Lipid	Long chain fatty acid
Oleate__18_1n9_	Yes	Lipid	Long chain fatty acid
Palmitate__16_0_	Yes	Lipid	Long chain fatty acid
Palmitoleate__16_1n7_	Yes	Lipid	Long chain fatty acid
Pentadecanoate__15_0_	Yes	Lipid	Long chain fatty acid
Stearate__18_0_	Yes	Lipid	Long chain fatty acid
Adrenate__22_4n6_	Yes	Lipid	Long chain fatty acid; polyunsaturated fatty acid (N3 and N6)
Arachidonate__20_4n6_	Yes	Lipid	Long chain fatty acid; polyunsaturated fatty acid (N3 and N6)
Dihomo_linoleate__20_2n6_	Yes	Lipid	Long chain fatty acid; polyunsaturated fatty acid (N3 and N6)
Docosadienoate__22_2n6_	Yes	Lipid	Long chain fatty acid; polyunsaturated fatty acid (N3 and N6)
Docosatrienoate	Yes	Lipid	Long chain fatty acid; polyunsaturated fatty acid (N3 and N6)
Stearidonate__18_4n3_	Yes	Lipid	Long chain fatty acid; polyunsaturated

			fatty acid (N3 and N6)
_1_arachidonoylglycerophoscho	Yes	Lipid	Lysolipid
_1_arachidonoylglycerophoseth	Yes	Lipid	Lysolipid
_1_arachidonoylglycerophosino	Yes	Lipid	Lysolipid
_1_linoleoylglycerophosphocho	Yes	Lipid	Lysolipid
_1_linoleoylglycerophosphoeth	Yes	Lipid	Lysolipid
_1_linoleoylglycerophosphoino	Yes	Lipid	Lysolipid
_1_oleoylglycerophosphocholin	Yes	Lipid	Lysolipid
_1_oleoylglycerophosphoethano	Yes	Lipid	Lysolipid
_1_oleoylglycerophosphoinosit	Yes	Lipid	Lysolipid
_1_palmitoleoylglycerophospho	Yes	Lipid	Lysolipid
_1_palmitoylglycerophosphocho	Yes	Lipid	Lysolipid
_1_palmitoylglycerophosphoeth	Yes	Lipid	Lysolipid
_1_palmitoylglycerophosphoino	Yes	Lipid	Lysolipid
_1_palmitoylplasmenylethanola	Yes	Lipid	Lysolipid
_1_stearoylglycerophosphochol	Yes	Lipid	Lysolipid
_1_stearoylglycerophosphoetha	Yes	Lipid	Lysolipid
_1_stearoylglycerophosphoinos	Yes	Lipid	Lysolipid
_2_palmitoylglycerophosphocho	Yes	Lipid	Lysolipid
_2_stearoylglycerophosphochol	Yes	Lipid	Lysolipid
_2_stearoylglycerophosphoetha	Yes	Lipid	Lysolipid
Stearoyl_linoleoyl_gppe_1	Yes	Lipid	Lysolipid
_10_undecenoate__11_1n1_	Yes	Lipid	Medium chain fatty acid
_5_dodecenoate__12_1n7_	Yes	Lipid	Medium chain fatty acid
Caprate__10_0_	Yes	Lipid	Medium chain fatty acid
Caproate__6_0_	Yes	Lipid	Medium chain fatty acid
Caprylate__8_0_	Yes	Lipid	Medium chain fatty acid
Heptanoate__7_0_	Yes	Lipid	Medium chain fatty acid
Laurate__12_0_	Yes	Lipid	Medium chain fatty acid
Pelargonate__9_0_	Yes	Lipid	Medium chain fatty acid
_1_arachidonylglycerol	Yes	Lipid	Monoacylglycerol
_1_linoleoylglycero	Yes	Lipid	Monoacylglycerol
_1_myristoylglycerol	Yes	Lipid	Monoacylglycerol
_1_oleoylglycero	Yes	Lipid	Monoacylglycerol
_1_palmitoylglycerol	Yes	Lipid	Monoacylglycerol
_1_pentadecanoylglycerol	Yes	Lipid	Monoacylglycerol
_1_stearoylglycero	Yes	Lipid	Monoacylglycerol
_2_linoleoylglycerol__2_monol	Yes	Lipid	Monoacylglycerol
_2_myristoylglycerol	Yes	Lipid	Monoacylglycerol
_2_palmitoylglycerol	Yes	Lipid	Monoacylglycerol
Cholate	Yes	Lipid	Primary bile acid metabolism
Glycochenodeoxycholate	Yes	Lipid	Primary bile acid metabolism
Glycocholate	Yes	Lipid	Primary bile acid metabolism

Taurochenodeoxycholate	Yes	Lipid	Primary bile acid metabolism
Taurocholate	Yes	Lipid	Primary bile acid metabolism
Glycocholenate_sulfate	Yes	Lipid	Secondary bile acid metabolism
Glycodeoxycholate	Yes	Lipid	Secondary bile acid metabolism
Glycohyocholate	Yes	Lipid	Secondary bile acid metabolism
Glycolithocholate_sulfate	Yes	Lipid	Secondary bile acid metabolism
Glycoursodeoxycholate	Yes	Lipid	Secondary bile acid metabolism
Taurocholenate_sulfate	Yes	Lipid	Secondary bile acid metabolism
Taurodeoxycholate	Yes	Lipid	Secondary bile acid metabolism
Taurolithocholate_3_sulfate	Yes	Lipid	Secondary bile acid metabolism
Tauroursodeoxycholate	Yes	Lipid	Secondary bile acid metabolism
Valerate	Yes	Lipid	Short chain fatty acid
Palmitoyl_sphingomyelin	Yes	Lipid	Sphingolipid metabolism
Sphinganine	Yes	Lipid	Sphingolipid metabolism
Sphingosine	Yes	Lipid	Sphingolipid metabolism
Stearoyl_sphingomyelin	Yes	Lipid	Sphingolipid metabolism
_21_hydroxypregnenolone_disul	Yes	Lipid	Sterol/steroid
_4_androsten_3beta_17beta_d_1	Yes	Lipid	Sterol/steroid
_4_androsten_3beta_17beta_d_2	Yes	Lipid	Sterol/steroid
_5a_androstan_3a_17bdd	Yes	Lipid	Sterol/steroid
_5alpha_androstan_3beta_17alp	Yes	Lipid	Sterol/steroid
_5alpha_androstan_3beta_17bet	Yes	Lipid	Sterol/steroid
_5alpha_pregnan_3beta_20add	Yes	Lipid	Sterol/steroid
_7_hoca	Yes	Lipid	Sterol/steroid
Andro_steroid_monosulfate_1	Yes	Lipid	Sterol/steroid
Androsterone_sulfate	Yes	Lipid	Sterol/steroid
Campesterol	Yes	Lipid	Sterol/steroid
Cholesterol	Yes	Lipid	Sterol/steroid
Corticosterone	Yes	Lipid	Sterol/steroid
Cortisol	Yes	Lipid	Sterol/steroid
Cortisone	Yes	Lipid	Sterol/steroid
Dhea_s	Yes	Lipid	Sterol/steroid
Epiandrosterone_sulfate	Yes	Lipid	Sterol/steroid
Lathosterol	Yes	Lipid	Sterol/steroid
Pregn_steroid_monosulfate	Yes	Lipid	Sterol/steroid
Pregnanediol_3_glucuronide	Yes	Lipid	Sterol/steroid
Pregnen_diol_disulfate	Yes	Lipid	Sterol/steroid
Pregnenolone_sulfate	Yes	Lipid	Sterol/steroid
Isovalerate	Yes	Lipid; amino acid	Fatty acid metabolism; valine, leucine and isoleucine metabolism
_1_2_propanediol	Yes	Lipid; xenobiotics	Chemical; ketone bodies
Hypoxanthine	Yes	Nucleotide	Purine metabolism, (hypo)xanthine/inosine containing

Inosine	Yes	Nucleotide	Purine metabolism, (hypo)xanthine/inosine containing
Xanthine	Yes	Nucleotide	Purine metabolism, (hypo)xanthine/inosine containing
Adenine	Yes	Nucleotide	Purine metabolism, adenine containing
Adenosine	Yes	Nucleotide	Purine metabolism, adenine containing
N1_methyladenosine	Yes	Nucleotide	Purine metabolism, adenine containing
N6_methyladenosine	Yes	Nucleotide	Purine metabolism, adenine containing
_7_methylguanine	Yes	Nucleotide	Purine metabolism, guanine containing
Guanosine	Yes	Nucleotide	Purine metabolism, guanine containing
N1_methylguanosine	Yes	Nucleotide	Purine metabolism, guanine containing
N2_n2_dimethylguanosine	Yes	Nucleotide	Purine metabolism, guanine containing
N6_carbamoylthreonyladenosine	Yes	Nucleotide	Purine metabolism, guanine containing; purine metabolism, adenine containing
Allantoin	Yes	Nucleotide	Purine metabolism, urate metabolism; purine metabolism, (hypo)xanthine/inosine containing
Urate	Yes	Nucleotide	Purine metabolism, urate metabolism; purine metabolism, (hypo)xanthine/inosine containing
Cytidine	Yes	Nucleotide	Pyrimidine metabolism, cytidine containing
_5_6_dihydrothymine	Yes	Nucleotide	Pyrimidine metabolism, thymine containing
_5_6_dihydrouracil	Yes	Nucleotide	Pyrimidine metabolism, uracil containing
_5_methyluridine__ribothymidi	Yes	Nucleotide	Pyrimidine metabolism, uracil containing
Pseudouridine	Yes	Nucleotide	Pyrimidine metabolism, uracil containing
Uridine	Yes	Nucleotide	Pyrimidine metabolism, uracil containing
Glutamine_leucine	Yes	Peptide	Dipeptide
Glycylleucine	Yes	Peptide	Dipeptide
Glycylvaline	Yes	Peptide	Dipeptide
Isoleucylglycine	Yes	Peptide	Dipeptide
Leucylglycine	Yes	Peptide	Dipeptide
Phenylalanylalanine	Yes	Peptide	Dipeptide
Phenylalanylglycine	Yes	Peptide	Dipeptide
Threonylphenylalanine	Yes	Peptide	Dipeptide
Adsgegdfxaegggvr	Yes	Peptide	Fibrinogen cleavage peptide
Dsgegdfxaegggvr	Yes	Peptide	Fibrinogen cleavage peptide
Gamma_glutamylalanine	Yes	Peptide	Gamma-glutamyl amino acid
Gamma_glutamylglutamate	Yes	Peptide	Gamma-glutamyl amino acid
Gamma_glutamylglutamine	Yes	Peptide	Gamma-glutamyl amino acid
Gamma_glutamylisoleucine	Yes	Peptide	Gamma-glutamyl amino acid
Gamma_glutamylleucine	Yes	Peptide	Gamma-glutamyl amino acid

Gamma_glutamylmethionine	Yes	Peptide	Gamma-glutamyl amino acid
Gamma_glutamylphenylalanine	Yes	Peptide	Gamma-glutamyl amino acid
Gamma_glutamylthreonine	Yes	Peptide	Gamma-glutamyl amino acid
Gamma_glutamyltryptophan	Yes	Peptide	Gamma-glutamyl amino acid
Gamma_glutamyltyrosine	Yes	Peptide	Gamma-glutamyl amino acid
Gamma_glutamylvaline	Yes	Peptide	Gamma-glutamyl amino acid
Bradykinin__des_arg_9_	Yes	Peptide	Polypeptide
Hwesasxx	Yes	Peptide	Polypeptide
Cys_gly__oxidized	Yes	Peptide; amino acid	Dipeptide derivative; glutathione metabolism
Pro_hydroxy_pro	Yes	Peptide; amino acid	Dipeptide; urea cycle; arginine and proline metabolism
_2_ethylphenylsulfate	Yes	Xenobiotics	Benzoate metabolism
_2_hydroxyhippurate__salicylu	Yes	Xenobiotics	Benzoate metabolism
_3_ethylphenylsulfate	Yes	Xenobiotics	Benzoate metabolism
_3_hydroxyhippurate	Yes	Xenobiotics	Benzoate metabolism
_3_methyl_catechol_sulfate_1	Yes	Xenobiotics	Benzoate metabolism
_3_methyl_catechol_sulfate_2	Yes	Xenobiotics	Benzoate metabolism
_4_ethylphenylsulfate	Yes	Xenobiotics	Benzoate metabolism
_4_hydroxyhippurate	Yes	Xenobiotics	Benzoate metabolism
_4_methylcatechol_sulfate	Yes	Xenobiotics	Benzoate metabolism
_4_vinylphenol_sulfate	Yes	Xenobiotics	Benzoate metabolism
Benzoate	Yes	Xenobiotics	Benzoate metabolism
Catechol_sulfate	Yes	Xenobiotics	Benzoate metabolism
Hippurate	Yes	Xenobiotics	Benzoate metabolism
O_methylcatechol_sulfate	Yes	Xenobiotics	Benzoate metabolism
_2_aminophenol_sulfate	Yes	Xenobiotics	Chemical
Glycolate__hydroxyacetate_	Yes	Xenobiotics	Chemical
_2_piperidinone	Yes	Xenobiotics	Chemical; food component/plant
Ethyl_glucuronide	Yes	Xenobiotics	Detoxification metabolism; chemical
_4_acetylphenol_sulfate	Yes	Xenobiotics	Drug
Atenolol	Yes	Xenobiotics	Drug
Hydroquinone_sulfate	Yes	Xenobiotics	Drug
Metoprolol_acid_metabolite	Yes	Xenobiotics	Drug
Salicylate	Yes	Xenobiotics	Drug
Salicyluric_glucuronide	Yes	Xenobiotics	Drug
Cinnamoylglycine	Yes	Xenobiotics	Food component/plant
Dihydroferulic_acid	Yes	Xenobiotics	Food component/plant
Ergothioneine	Yes	Xenobiotics	Food component/plant
Homostachydrine	Yes	Xenobiotics	Food component/plant
N__2_furoyl_glycine	Yes	Xenobiotics	Food component/plant
Piperine	Yes	Xenobiotics	Food component/plant
Quinate	Yes	Xenobiotics	Food component/plant
Saccharin	Yes	Xenobiotics	Food component/plant

Solanidine	Yes	Xenobiotics	Food component/plant
Stachydrine	Yes	Xenobiotics	Food component/plant
Thymol_sulfate	Yes	Xenobiotics	Food component/plant
Erythritol	Yes	Xenobiotics	Sugar, sugar substitute, starch; food component/plant
_3_hydroxycotinine_glucuronid	Yes	Xenobiotics	Tobacco metabolite
Cotinine	Yes	Xenobiotics	Tobacco metabolite
Cotinine_n_oxide	Yes	Xenobiotics	Tobacco metabolite
Hydroxycotinine	Yes	Xenobiotics	Tobacco metabolite
_1_3_7_trimethylurate	Yes	Xenobiotics	Xanthine metabolism
_1_3_dimethylurate	Yes	Xenobiotics	Xanthine metabolism
_1_7_dimethylurate	Yes	Xenobiotics	Xanthine metabolism
_1_methylurate	Yes	Xenobiotics	Xanthine metabolism
_1_methylxanthine	Yes	Xenobiotics	Xanthine metabolism
_3_7_dimethylurate	Yes	Xenobiotics	Xanthine metabolism
_3_methylxanthine	Yes	Xenobiotics	Xanthine metabolism
_5_acetylamino_6_amino_3_meth	Yes	Xenobiotics	Xanthine metabolism
_5_acetylamino_6_formylamino_	Yes	Xenobiotics	Xanthine metabolism
_7_methylxanthine	Yes	Xenobiotics	Xanthine metabolism
Caffeine	Yes	Xenobiotics	Xanthine metabolism
Paraxanthine	Yes	Xenobiotics	Xanthine metabolism
Theophylline	Yes	Xenobiotics	Xanthine metabolism
N_acetylaspartate__naa_	No	Amino acid	Alanine and aspartate metabolism
Guanidinoacetate	No	Amino acid	Creatine metabolism
Alpha_ketobutyrate	No	Amino acid	Cysteine, methionine, sam, taurine metabolism
Cysteine_s_sulfate	No	Amino acid	Cysteine, methionine, sam, taurine metabolism
Hypotaurine	No	Amino acid	Cysteine, methionine, sam, taurine metabolism
Methionine_sulfone	No	Amino acid	Cysteine, methionine, sam, taurine metabolism
Methionine_sulfoxide	No	Amino acid	Cysteine, methionine, sam, taurine metabolism
N_acetyltaurine	No	Amino acid	Cysteine, methionine, sam, taurine metabolism
S_adenosylhomocysteine__sah_	No	Amino acid	Cysteine, methionine, sam, taurine metabolism
N_acetylglutamate	No	Amino acid	Glutamate metabolism
N_acetylglutamine	No	Amino acid	Glutamate metabolism
Naag	No	Amino acid	Glutamate metabolism
Glutathione__reduced__gsh_	No	Amino acid	Glutathione metabolism
_2_phenylglycine	No	Amino acid	Glycine, serine and threonine metabolism
Beta_hydroxypyruvate	No	Amino acid	Glycine, serine and threonine metabolism

Sarcosine__n_methylglycine_	No	Amino acid	Glycine, serine and threonine metabolism
Guanidinosuccinate	No	Amino acid	Guanidino and acetamido metabolism
_4_imidazoleacetate	No	Amino acid	Histidine metabolism
Hydantoin_5_propionic_acid	No	Amino acid	Histidine metabolism
Imidazole_lactate	No	Amino acid	Histidine metabolism
N_acetyl_1_methylhistidine	No	Amino acid	Histidine metabolism
N_acetyl_3_methylhistidine	No	Amino acid	Histidine metabolism
N_acetylhistidine	No	Amino acid	Histidine metabolism
_3_methylglutarylcarnitine_1	No	Amino acid	Lysine metabolism
_3_methylglutarylcarnitine_2	No	Amino acid	Lysine metabolism
_6_oxopiperidine_2_carboxylic	No	Amino acid	Lysine metabolism
Glutarate__pentanedioate_	No	Amino acid	Lysine metabolism
N_6_trimethyllysine	No	Amino acid	Lysine metabolism
N2_acetyllysine	No	Amino acid	Lysine metabolism
_3_methylglutaconate	No	Amino acid	Lysine metabolism; valine, leucine and isoleucine metabolism
_3__3__sulfooxy_phenyl_propan	No	Amino acid	Phenylalanine & tyrosine metabolism
_3__4_hydroxyphenyl_propionat	No	Amino acid	Phenylalanine & tyrosine metabolism
_3_4_dimethoxy_hydrocinnamic	No	Amino acid	Phenylalanine & tyrosine metabolism
_3_methoxytyramine_sulfate	No	Amino acid	Phenylalanine & tyrosine metabolism
_4_hydroxyphenylacetate	No	Amino acid	Phenylalanine & tyrosine metabolism
_5_hydroxymethyl_2_furoic_aci	No	Amino acid	Phenylalanine & tyrosine metabolism
Dopamine_sulfate_1	No	Amino acid	Phenylalanine & tyrosine metabolism
Dopamine_sulfate_2	No	Amino acid	Phenylalanine & tyrosine metabolism
Homovanillate__hva_	No	Amino acid	Phenylalanine & tyrosine metabolism
N_formylphenylalanine	No	Amino acid	Phenylalanine & tyrosine metabolism
P_cresol_glucuronide	No	Amino acid	Phenylalanine & tyrosine metabolism
Phenylacetylcarnitine	No	Amino acid	Phenylalanine & tyrosine metabolism
Phenylpyruvate	No	Amino acid	Phenylalanine & tyrosine metabolism
Thyroxine	No	Amino acid	Phenylalanine & tyrosine metabolism
Tyramine_o_sulfate	No	Amino acid	Phenylalanine & tyrosine metabolism
Vanillylmandelate__vma_	No	Amino acid	Phenylalanine & tyrosine metabolism
_5_hydroxyindoleacetate	No	Amino acid	Tryptophan metabolism
Indole_3_carboxylic_acid	No	Amino acid	Tryptophan metabolism
Indolebutyrate	No	Amino acid	Tryptophan metabolism
Indolepyruvate	No	Amino acid	Tryptophan metabolism
N_acetylkynurenine_2	No	Amino acid	Tryptophan metabolism
Picolinate	No	Amino acid	Tryptophan metabolism
Serotonin__5ht_	No	Amino acid	Tryptophan metabolism
Xanthurenate	No	Amino acid	Tryptophan metabolism
Homoarginine	No	Amino acid	Urea cycle; arginine and proline metabolism
N_acetylarginine	No	Amino acid	Urea cycle; arginine and proline

			metabolism
N_acetylcitrulline	No	Amino acid	Urea cycle; arginine and proline metabolism
N_methylproline	No	Amino acid	Urea cycle; arginine and proline metabolism
N2_n5_diacetylornithine	No	Amino acid	Urea cycle; arginine and proline metabolism
Proline	No	Amino acid	Urea cycle; arginine and proline metabolism
_2_methylbutyroylcarnitine	No	Amino acid	Valine, leucine and isoleucine metabolism
_2_methylbutyrylcarnitine	No	Amino acid	Valine, leucine and isoleucine metabolism
_2_methylbutyrylglycine	No	Amino acid	Valine, leucine and isoleucine metabolism
_3_methylcrotonylglycine	No	Amino acid	Valine, leucine and isoleucine metabolism
Allo_isoleucine	No	Amino acid	Valine, leucine and isoleucine metabolism
Alpha_hydroxyisovaleroyl_carn	No	Amino acid	Valine, leucine and isoleucine metabolism
Beta_hydroxyisovaleroylcarnit	No	Amino acid	Valine, leucine and isoleucine metabolism
Hydroxyisovaleroyl_carnitine	No	Amino acid	Valine, leucine and isoleucine metabolism
Isobutyrylglycine	No	Amino acid	Valine, leucine and isoleucine metabolism
Methylsuccinate	No	Amino acid	Valine, leucine and isoleucine metabolism
Tigloylglycine	No	Amino acid	Valine, leucine and isoleucine metabolism
N_oleoyltaurine	No	Amino acid; lipid	Cysteine, methionine, sam, taurine metabolism; endocannabinoid
Oleoyltaurine	No	Amino acid; lipid	Cysteine, methionine, sam, taurine metabolism; endocannabinoid
Methyl_indole_3_acetate	No	Amino acid; xenobiotics	Tryptophan metabolism; food component/plant
_2_hydroxyisobutyrate	No	Amino acid; xenobiotics	Valine, leucine and isoleucine metabolism; chemical
N_acetylneuraminate	No	Carbohydrate	Aminosugar metabolism
Glucuronate	No	Carbohydrate	Aminosugars metabolism; glycolysis, gluconeogenesis, pyruvate metabolism
Sucrose	No	Carbohydrate	Disaccharides and oligosaccharides; fructose, mannose, galactose, starch, and sucrose metabolism
Galactonate	No	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism
Methyl_beta_glucopyranoside	No	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism
Sorbitol	No	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism

Sorbose	No	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism
Isomaltose	No	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism; glycogen metabolism
Maltose	No	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism; glycogen metabolism
Maltotriose	No	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism; glycogen metabolism
Maltotetraose	No	Carbohydrate	Glycogen metabolism
_1_3_dihydroxyacetone	No	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism
Ribonate	No	Carbohydrate	Pentose metabolism
Xylulose	No	Carbohydrate	Pentose metabolism
Erythrulose	No	Carbohydrate; secondary metabolism	Advanced glycation end-product
Gulonic_acid	No	Cofactors and vitamins	Ascorbate and aldarate metabolism
Bilirubin__e_z_or_z_e_	No	Cofactors and vitamins	Hemoglobin and porphyrin metabolism
l_urobilinogen	No	Cofactors and vitamins	Hemoglobin and porphyrin metabolism
_1_methylnicotinamide	No	Cofactors and vitamins	Nicotinate and nicotinamide metabolism
Nicotinate	No	Cofactors and vitamins	Nicotinate and nicotinamide metabolism
Quinolinate	No	Cofactors and vitamins	Nicotinate and nicotinamide metabolism
Pyridoxal	No	Cofactors and vitamins	Pyridoxal metabolism; vitamin b6 metabolism
Flavin_adenine_dinucleotide	No	Cofactors and vitamins	Riboflavin metabolism
Biopterin	No	Cofactors and vitamins	Tetrahydrobiopterin metabolism
Alpha_cehc	No	Cofactors and vitamins	Tocopherol metabolism
Alpha_cehc_glucuronide	No	Cofactors and vitamins	Tocopherol metabolism
Alpha_cehc_sulfate	No	Cofactors and vitamins	Tocopherol metabolism
_2_3_dihydroxyisovalerate	No	Cofactors and vitamins; xenobiotics	Pantothenate and coa metabolism; food component/plant
_2_methylcitrate	No	Energy	Krebs cycle / tca cycle
Aconitate__cis_or_trans_	No	Energy	Krebs cycle / tca cycle
Itaconate__methylenesuccinate	No	Energy	Krebs cycle / tca cycle
Acetylphosphate	No	Energy	Oxidative phosphorylation

Pyrophosphate__ppi_	No	Energy	Oxidative phosphorylation
_1_dihomo_linoleoylglyceropho	No	Lipid	
_1_eicosadienoylglycerophosph	No	Lipid	
_1_gamma_linolenoylglycerol	No	Lipid	
_1_heptadecanoylglycerophosph	No	Lipid	
_1_margaroylglycerophosphocho	No	Lipid	
_1_margaroylglycerophosphoeth	No	Lipid	
_3_methylglutarylcarnitine	No	Lipid	
Hexenedioylcarnitine	No	Lipid	
Hyocholate	No	Lipid	
_3_dehydrocarnitine	No	Lipid	Carnitine metabolism
Linoleoylcarnitine	No	Lipid	Carnitine metabolism
Myristoleoylcarnitine	No	Lipid	Carnitine metabolism
_2_methylmalonyl_carnitine	No	Lipid	Carnitine metabolism; fatty acid synthesis
_20_hete	No	Lipid	Eicosanoid
_5_hepe	No	Lipid	Eicosanoid
_5_hete	No	Lipid	Eicosanoid
_5_oxoete	No	Lipid	Eicosanoid
Leukotriene_b4	No	Lipid	Eicosanoid
Thromboxane_b2	No	Lipid	Eicosanoid
N_palmitoyl_taurine	No	Lipid	Endocannabinoid
N_palmitoyltaurine	No	Lipid	Endocannabinoid
N_stearoyl_taurine	No	Lipid	Endocannabinoid
N_stearoyltaurine	No	Lipid	Endocannabinoid
Butyrylglycine	No	Lipid	Fatty acid metabolism (also bcaa metabolism)
Propionylglycine	No	Lipid	Fatty acid metabolism (also bcaa metabolism)
Hexanoylglycine	No	Lipid	Fatty acid metabolism(acyl glycine)
N_linoleoylglycine	No	Lipid	Fatty acid metabolism(acyl glycine)
N_octanoylglycine	No	Lipid	Fatty acid metabolism(acyl glycine)
N_palmitoyl_glycine	No	Lipid	Fatty acid metabolism(acyl glycine)
Malonylcarnitine	No	Lipid	Fatty acid synthesis
Stearamide	No	Lipid	Fatty acid, amide
_13_methylmyristic_acid	No	Lipid	Fatty acid, branched
Pristanate	No	Lipid	Fatty acid, branched
_1_11_undecanedicarboxylate	No	Lipid	Fatty acid, dicarboxylate
Adipate	No	Lipid	Fatty acid, dicarboxylate
Eicosanodioate	No	Lipid	Fatty acid, dicarboxylate
Maleate__cis_butenedioate_	No	Lipid	Fatty acid, dicarboxylate
Pimelate__heptanedioate_	No	Lipid	Fatty acid, dicarboxylate
Suberate__octanedioate_	No	Lipid	Fatty acid, dicarboxylate
_12_13_dihome	No	Lipid	Fatty acid, dihydroxy

_9_10_dihome	No	Lipid	Fatty acid, dihydroxy
Methyl_linoleate	No	Lipid	Fatty acid, methyl ester
Methyl_stearate	No	Lipid	Fatty acid, methyl ester
Palmitate__methyl_ester	No	Lipid	Fatty acid, methyl ester
_16_hydroxypalmitate	No	Lipid	Fatty acid, monohydroxy
_2_hydroxydecanoate	No	Lipid	Fatty acid, monohydroxy
_2_hydroxydecanoic_acid	No	Lipid	Fatty acid, monohydroxy
_2_hydroxymyristate	No	Lipid	Fatty acid, monohydroxy
_3_hydroxylaurate	No	Lipid	Fatty acid, monohydroxy
_3_hydroxymyristate	No	Lipid	Fatty acid, monohydroxy
_3_hydroxypalmitate	No	Lipid	Fatty acid, monohydroxy
_3_hydroxysebacate	No	Lipid	Fatty acid, monohydroxy
_5_hydroxyhexanoate	No	Lipid	Fatty acid, monohydroxy
_8_hydroxyoctanoate	No	Lipid	Fatty acid, monohydroxy
_9_hydroxystearate	No	Lipid	Fatty acid, monohydroxy
Alpha_hydroxycaproate	No	Lipid	Fatty acid, monohydroxy
_9_10_epoxystearate	No	Lipid	Fatty acid, oxidized
Choline_phosphate	No	Lipid	Glycerolipid metabolism; phospholipid metabolism
Glycerophosphoethanolamine	No	Lipid	Glycerolipid metabolism; phospholipid metabolism
_1_oleoylglycerophosphoglycer	No	Lipid	Glycerophosphodiester / lysolipid
_1_palmitoylglycerophosphogly	No	Lipid	Glycerophosphodiester / lysolipid
Scyllo_inositol	No	Lipid	Inositol metabolism
_4_hydroxy_2_nonenal	No	Lipid	Lipid peroxidation; fatty acid, oxidized
Arachidate__20_0_	No	Lipid	Long chain fatty acid
Cis_vaccenate__18_1n7_	No	Lipid	Long chain fatty acid
Erucate__22_1n9_	No	Lipid	Long chain fatty acid
Mead_acid__20_3n9_	No	Lipid	Long chain fatty acid; polyunsaturated fatty acid (n3 and n6)
_1_arachidonoyl_lpa	No	Lipid	Lysolipid
_1_arachidonoylglyercophospha	No	Lipid	Lysolipid
_1_arachidoylglycerophosphoch	No	Lipid	Lysolipid
_1_docosahexaenoylglyceropeth	No	Lipid	Lysolipid
_1_docosahexaenoylglycerophos	No	Lipid	Lysolipid
_1_docosapentaenoylglyceropho	No	Lipid	Lysolipid
_1_eicosapentaenoylglyceropet	No	Lipid	Lysolipid
_1_eicosapentaenoylglyceropho	No	Lipid	Lysolipid
_1_eicosatrienoylglycerophosp	No	Lipid	Lysolipid
_1_eicosatrienoylglyceroppeth	No	Lipid	Lysolipid
_1_eicosenoylglycerophosphoch	No	Lipid	Lysolipid
_1_eicosenoylglycerophosphoet	No	Lipid	Lysolipid
_1_linolenoylglycerophosphoch	No	Lipid	Lysolipid
_1_linolenoylglycerophosphoet	No	Lipid	Lysolipid

_1_myristoleoylglycerophospho	No	Lipid	Lysolipid
_1_myristoylglycerophosphocho	No	Lipid	Lysolipid
_1_nonadecanoylglycerophospho	No	Lipid	Lysolipid
_1_oleoylglycerophosphate	No	Lipid	Lysolipid
_1_oleoylplasmenylethanolamin	No	Lipid	Lysolipid
_1_palmitoleoylglyceropea	No	Lipid	Lysolipid
_1_palmitoleoylglyceropin	No	Lipid	Lysolipid
_1_palmitoylglycerophosphate	No	Lipid	Lysolipid
_1_pentadecanoylglycerophosph	No	Lipid	Lysolipid
_1_stearoylglycerophosphate	No	Lipid	Lysolipid
_1_stearoylglycerophosphoglyc	No	Lipid	Lysolipid
_1_stearoylglycerophosphoseri	No	Lipid	Lysolipid
_1_stearoylplasmenylethanolam	No	Lipid	Lysolipid
_2_arachidonoylglycerophoscho	No	Lipid	Lysolipid
_2_arachidonoylglycerophoseth	No	Lipid	Lysolipid
_2_arachidonoylglycerophosino	No	Lipid	Lysolipid
_2_arachidoylglycerophosphoch	No	Lipid	Lysolipid
_2_docosahexaenoylglyceropc	No	Lipid	Lysolipid
_2_docosahexaenoylglycerope	No	Lipid	Lysolipid
_2_docosapentaenoylglycerope	No	Lipid	Lysolipid
_2_eicosapentaenoylglycerope	No	Lipid	Lysolipid
_2_eicosatrienoylglycerophosc	No	Lipid	Lysolipid
_2_linolenoylglycerophosphoch	No	Lipid	Lysolipid
_2_linoleoylglycerophosphocho	No	Lipid	Lysolipid
_2_linoleoylglycerophosphoeth	No	Lipid	Lysolipid
_2_myristoylglycerophosphocho	No	Lipid	Lysolipid
_2_oleoylglycerophosphocholin	No	Lipid	Lysolipid
_2_oleoylglycerophosphoethano	No	Lipid	Lysolipid
_2_oleoylglycerophosphoinosit	No	Lipid	Lysolipid
_2_palmitoleoylglycerophospho	No	Lipid	Lysolipid
_2_palmitoylglycerophosphoeth	No	Lipid	Lysolipid
_2_stearoylglycerophosphoinos	No	Lipid	Lysolipid
Palmitoyl_arachidonoyl_gppc_1	No	Lipid	Lysolipid
Palmitoyl_arachidonoyl_gppc_2	No	Lipid	Lysolipid
Palmitoyl_linoleoyl_gppc_1	No	Lipid	Lysolipid
Palmitoyl_linoleoyl_gppc_2	No	Lipid	Lysolipid
Palmitoyl_linoleoyl_gppi_1	No	Lipid	Lysolipid
Palmitoyl_oleoyl_gppc_1	No	Lipid	Lysolipid
Palmitoyl_oleoyl_gppg_2	No	Lipid	Lysolipid
Palmitoyl_palmitoyl_gppc_1	No	Lipid	Lysolipid
Palmitoyl_palmitoyl_gppc_2	No	Lipid	Lysolipid
Stearoyl_arachidonoyl_gppc_1	No	Lipid	Lysolipid
Stearoyl_arachidonoyl_gppc_2	No	Lipid	Lysolipid

Stearoyl_arachidonoyl_gppe_1	No	Lipid	Lysolipid
Stearoyl_arachidonoyl_gppi_1	No	Lipid	Lysolipid
Stearoyl_linoleoyl_gppc_1	No	Lipid	Lysolipid
Stearoyl_linoleoyl_gppc_2	No	Lipid	Lysolipid
_2_aminoheptanoate	No	Lipid	Medium chain fatty acid; fatty acid, amino
_3_hydroxy_3_methylglutarate	No	Lipid	Mevalonate metabolism
_1_dihomo_linolenylglycerol__	No	Lipid	Monoacylglycerol
_1_docosahexaenoylglycerol	No	Lipid	Monoacylglycerol
_1_linolenoylglycerol	No	Lipid	Monoacylglycerol
_2_arachidonoyl_glycerol	No	Lipid	Monoacylglycerol
_2_docosahexaenoylglcyerol	No	Lipid	Monoacylglycerol
_2_oleoylglycerol__2_monoolei	No	Lipid	Monoacylglycerol
Chenodeoxycholate	No	Lipid	Primary bile acid metabolism
Tauro_beta_muricholate	No	Lipid	Primary bile acid metabolism
Pregnanolone_allopregnanolone	No	Lipid	Progestin steroids
_3b_hydroxy_5_cholenoic_acid	No	Lipid	Secondary bile acid metabolism
_3beta_7alpha_dihydroxy_5_cho	No	Lipid	Secondary bile acid metabolism
_7_ketodeoxycholate	No	Lipid	Secondary bile acid metabolism
Deoxycholate	No	Lipid	Secondary bile acid metabolism
Glycohyodeoxycholic_acid	No	Lipid	Secondary bile acid metabolism
Glycolithocholate	No	Lipid	Secondary bile acid metabolism
Taurolithocholate	No	Lipid	Secondary bile acid metabolism
Ursodeoxycholate	No	Lipid	Secondary bile acid metabolism
_3_methyladipate	No	Lipid	Short chain fatty acid; fatty acid, dicarboxylate
Arachidoyl_sphingomyelin	No	Lipid	Sphingolipid metabolism
Eicosenoyl_sphingomyelin	No	Lipid	Sphingolipid metabolism
Erythro_sphingosine_1_phospha	No	Lipid	Sphingolipid metabolism
Euricoyl_sphingomyelin	No	Lipid	Sphingolipid metabolism
Myristoleoyl_sphingomyelin	No	Lipid	Sphingolipid metabolism
Myristoyl_sphingomyelin	No	Lipid	Sphingolipid metabolism
Nervonoyl_sphingomyelin	No	Lipid	Sphingolipid metabolism
Oleoyl_sphingomyelin	No	Lipid	Sphingolipid metabolism
Palmitoleoyl_sphingomyelin	No	Lipid	Sphingolipid metabolism
Sphingosine_1_phosphate	No	Lipid	Sphingolipid metabolism
Sphingosyl_phosphocholine	No	Lipid	Sphingolipid metabolism
_11_dehydrocorticosterone	No	Lipid	Sterol/steroid
_11_ketoetiocholanolone_glucu	No	Lipid	Sterol/steroid
_16a_hydroxy_dhea_3_sulfate	No	Lipid	Sterol/steroid
_17alpha_hydroxypregnanolone	No	Lipid	Sterol/steroid
_21_hydroxypregnenolone_mono2	No	Lipid	Sterol/steroid
_21_hydroxypregnenolone_monos	No	Lipid	Sterol/steroid
_4_androsten_3alpha_17adm_2	No	Lipid	Sterol/steroid

_4_androsten_3alpha_17adm_3	No	Lipid	Sterol/steroid
_4_androsten_3beta_17bdm_1	No	Lipid	Sterol/steroid
_4_androsten_3beta_17bdm_2	No	Lipid	Sterol/steroid
_5_pregnen_3b__17_d_20_o_3_s	No	Lipid	Sterol/steroid
_5a_androstan_3a_17add	No	Lipid	Sterol/steroid
_5a_androstan_3a_17adm	No	Lipid	Sterol/steroid
_5a_androstan_3a_17bdm1	No	Lipid	Sterol/steroid
_5a_androstan_3a_17bdm2	No	Lipid	Sterol/steroid
_5a_androstan_3b_17bdm1	No	Lipid	Sterol/steroid
_5a_androstan_3b_17bdm2	No	Lipid	Sterol/steroid
_5alpha_pregnan_3alpha_20bdd1	No	Lipid	Sterol/steroid
_5alpha_pregnan_3aorb_20bdd	No	Lipid	Sterol/steroid
_5alpha_pregnan_3beta_20adm2	No	Lipid	Sterol/steroid
_5alpha_pregnan_3beta_20bdm1	No	Lipid	Sterol/steroid
_7_alpha_hydroxycholesterol	No	Lipid	Sterol/steroid
_7_beta_hydroxycholesterol	No	Lipid	Sterol/steroid
_7_dehydrocholesterol	No	Lipid	Sterol/steroid
Beta_sitosterol	No	Lipid	Sterol/steroid
Estrone_3_sulfate	No	Lipid	Sterol/steroid
Etiocholanolone_glucuronide	No	Lipid	Sterol/steroid
Testosterone	No	Lipid	Sterol/steroid
Testosterone_sulfate	No	Lipid	Sterol/steroid
Ethylmalonate	No	Lipid; amino acid	Carnitine metabolism; valine, leucine and isoleucine metabolism
Methylphosphate	No	Nucleotide	Purine and pyrimidine metabolism
Xanthosine	No	Nucleotide	Purine metabolism, (hypo)xanthine/inosine containing
Adenosine_5__monophosphate__a	No	Nucleotide	Purine metabolism, adenine containing
Camp	No	Nucleotide	Purine metabolism, adenine containing
N6_succinyladenosine	No	Nucleotide	Purine metabolism, adenine containing
Guanine	No	Nucleotide	Purine metabolism, guanine containing
N2_methylguanosine	No	Nucleotide	Purine metabolism, guanine containing
N4_acetylcytidine	No	Nucleotide	Pyrimidine metabolism, cytidine containing
Dihydroorotate	No	Nucleotide	Pyrimidine metabolism, orotate containing
Orotate	No	Nucleotide	Pyrimidine metabolism, orotate containing
Orotidine	No	Nucleotide	Pyrimidine metabolism, orotate containing
_3_aminoisobutyrate	No	Nucleotide	Pyrimidine metabolism, thymine containing; valine, leucine and isoleucine metabolism
_2__deoxyuridine	No	Nucleotide	Pyrimidine metabolism, uracil containing
Uracil	No	Nucleotide	Pyrimidine metabolism, uracil

			containing
Alanylalanine	No	Peptide	Dipeptide
Alanylleucine	No	Peptide	Dipeptide
Alanylphenylalanine	No	Peptide	Dipeptide
Alpha_glutamyltyrosine	No	Peptide	Dipeptide
Arginylisoleucine	No	Peptide	Dipeptide
Arginylleucine	No	Peptide	Dipeptide
Arginylphenylalanine	No	Peptide	Dipeptide
Asparagylleucine	No	Peptide	Dipeptide
Aspartylleucine	No	Peptide	Dipeptide
Aspartylphenylalanine	No	Peptide	Dipeptide
Cyclo_gly_pro_	No	Peptide	Dipeptide
Cyclo_l_phe_d_pro_	No	Peptide	Dipeptide
Cyclo_leu_pro_	No	Peptide	Dipeptide
Glutamine_isoleucine	No	Peptide	Dipeptide
Glycylglycine	No	Peptide	Dipeptide
Glycylisoleucine	No	Peptide	Dipeptide
Glycylphenylalanine	No	Peptide	Dipeptide
Glycylproline	No	Peptide	Dipeptide
Histidylalanine	No	Peptide	Dipeptide
Histidylisoleucine	No	Peptide	Dipeptide
Histidylleucine	No	Peptide	Dipeptide
Histidylphenylalanine	No	Peptide	Dipeptide
Histidyltryptophan	No	Peptide	Dipeptide
Histidylvaline	No	Peptide	Dipeptide
Isoleucylalanine	No	Peptide	Dipeptide
Isoleucylasparagine	No	Peptide	Dipeptide
Isoleucylaspartate	No	Peptide	Dipeptide
Isoleucylisoleucine	No	Peptide	Dipeptide
Isoleucylleucine	No	Peptide	Dipeptide
Isoleucylphenylalanine	No	Peptide	Dipeptide
Isoleucylthreonine	No	Peptide	Dipeptide
Isoleucylvaline	No	Peptide	Dipeptide
Leucylalanine	No	Peptide	Dipeptide
Leucylarginine	No	Peptide	Dipeptide
Leucylasparagine	No	Peptide	Dipeptide
Leucylaspartate	No	Peptide	Dipeptide
Leucylglutamate	No	Peptide	Dipeptide
Leucylglutamine	No	Peptide	Dipeptide
Leucylleucine	No	Peptide	Dipeptide
Leucylphenylalanine	No	Peptide	Dipeptide
Leucylserine	No	Peptide	Dipeptide
Lysylmethionine	No	Peptide	Dipeptide

Lysylproline	No	Peptide	Dipeptide
Lysylvaline	No	Peptide	Dipeptide
Phenylalanylarginine	No	Peptide	Dipeptide
Phenylalanylglutamate	No	Peptide	Dipeptide
Phenylalanylleucine	No	Peptide	Dipeptide
Phenylalanylmethionine	No	Peptide	Dipeptide
Phenylalanylphenylalanine	No	Peptide	Dipeptide
Phenylalanylproline	No	Peptide	Dipeptide
Phenylalanylserine	No	Peptide	Dipeptide
Phenylalanyltryptophan	No	Peptide	Dipeptide
Phenylalanylvaline	No	Peptide	Dipeptide
Prolylalanine	No	Peptide	Dipeptide
Prolylglycine	No	Peptide	Dipeptide
Prolylphenylalanine	No	Peptide	Dipeptide
Pyroglutamylglutamine	No	Peptide	Dipeptide
Pyroglutamylglycine	No	Peptide	Dipeptide
Pyroglutamylvaline	No	Peptide	Dipeptide
Serylalanine	No	Peptide	Dipeptide
Serylleucine	No	Peptide	Dipeptide
Serylphenyalanine	No	Peptide	Dipeptide
Seryltyrosine	No	Peptide	Dipeptide
Threonylisoleucine	No	Peptide	Dipeptide
Threonylleucine	No	Peptide	Dipeptide
Tryptophylasparagine	No	Peptide	Dipeptide
Tryptophylaspartate	No	Peptide	Dipeptide
Tryptophylglutamate	No	Peptide	Dipeptide
Tryptophylglycine	No	Peptide	Dipeptide
Tryptophylleucine	No	Peptide	Dipeptide
Tryptophylmethionine	No	Peptide	Dipeptide
Tryptophylphenylalanine	No	Peptide	Dipeptide
Tryptophyltryptophan	No	Peptide	Dipeptide
Tyrosylalanine	No	Peptide	Dipeptide
Tyrosylglutamate	No	Peptide	Dipeptide
Tyrosylglutamine	No	Peptide	Dipeptide
Tyrosylglycine	No	Peptide	Dipeptide
Tyrosylisoleucine	No	Peptide	Dipeptide
Tyrosylleucine	No	Peptide	Dipeptide
Valylalanine	No	Peptide	Dipeptide
Valylarginine	No	Peptide	Dipeptide
Valylaspartate	No	Peptide	Dipeptide
Valylglutamate	No	Peptide	Dipeptide
Valylglutamine	No	Peptide	Dipeptide
Valylglycine	No	Peptide	Dipeptide

Valylhistidine	No	Peptide	Dipeptide
Valylisoleucine	No	Peptide	Dipeptide
Valylleucine	No	Peptide	Dipeptide
Valylphenylalanine	No	Peptide	Dipeptide
Valylserine	No	Peptide	Dipeptide
Valylvaline	No	Peptide	Dipeptide
N_acetylcarnosine	No	Peptide	Dipeptide derivative
Adpsgegdfxaegggvr	No	Peptide	Fibrinogen cleavage peptide
Gamma_glutamyl_2_aminobutyrat	No	Peptide	Gamma-glutamyl amino acid
Gamma_glutamylglycine	No	Peptide	Gamma-glutamyl amino acid
Gamma_glutamylhistidine	No	Peptide	Gamma-glutamyl amino acid
Gamma_glutamyllysine	No	Peptide	Gamma-glutamyl amino acid
Bradykinin	No	Peptide	Polypeptide
Hxgxa	No	Peptide	Polypeptide
_1_methyl_2_piperidinecarboxy	No	Unknown	
_3_hydroxyindolin_2_one	No	Unknown	
Tartronate__hydroxymalonate_	No	Xenobiotics	Bacterial/fungal
_3_methoxycatechol_sulfate_1	No	Xenobiotics	Benzoate metabolism
_3_methoxycatechol_sulfate_2	No	Xenobiotics	Benzoate metabolism
Methyl_4_hydroxybenzoate	No	Xenobiotics	Benzoate metabolism
Methyl_4_hydroxybenzoate_sulf	No	Xenobiotics	Benzoate metabolism
Propyl_4_hydroxybenzoate_sulf	No	Xenobiotics	Benzoate metabolism
_3_methoxybenzenepropanoic_ac	No	Xenobiotics	Benzoate metabolism; bacterial
_3__2_hydroxyphenyl_propionat	No	Xenobiotics	Benzoate metabolism; chemical
_1_2_3_benzenetriol_sulfate_2	No	Xenobiotics	Chemical
_2_ethylhexanoate	No	Xenobiotics	Chemical
_2_methyoxyresorcinol_sulfate	No	Xenobiotics	Chemical
_2_pyrrolidinone	No	Xenobiotics	Chemical
_3_hydroxypyridine_sulfate	No	Xenobiotics	Chemical
_4_hydroxychlorothalonil	No	Xenobiotics	Chemical
_4_methylbenzenesulfonate	No	Xenobiotics	Chemical
Dimethyl_sulfone	No	Xenobiotics	Chemical
Ectoine	No	Xenobiotics	Chemical
Glycerol_2_phosphate	No	Xenobiotics	Chemical
Heptaethylene_glycol	No	Xenobiotics	Chemical
Hexaethylene_glycol	No	Xenobiotics	Chemical
N_methylpipecolate	No	Xenobiotics	Chemical
Nornicotine	No	Xenobiotics	Chemical
O_sulfo_l_tyrosine	No	Xenobiotics	Chemical
Octaethylene_glycol	No	Xenobiotics	Chemical
Pentaethylene_glycol	No	Xenobiotics	Chemical
Phenylcarnitine	No	Xenobiotics	Chemical
S__3_hydroxypropyl_mercapturi	No	Xenobiotics	Chemical

Sulfate	No	Xenobiotics	Chemical
Tetraethylene_glycol	No	Xenobiotics	Chemical
Triethanolamine	No	Xenobiotics	Chemical
_1_hydroxy_2_naphthalenecarbo	No	Xenobiotics	Drug
_2_acetamidophenol_sulfate	No	Xenobiotics	Drug
_2_hydroxyacetaminophen_sulfa	No	Xenobiotics	Drug
_2_hydroxyibuprofen	No	Xenobiotics	Drug
_2_methoxyacetaminophen_glucu	No	Xenobiotics	Drug
_3__cystein_s_yl_acetaminophe	No	Xenobiotics	Drug
_3__n_acetyl_l_cystein_s_yl_	No	Xenobiotics	Drug
_3_hydroxyquinine	No	Xenobiotics	Drug
_4_acetamidophenol	No	Xenobiotics	Drug
_4_acetamidophenylglucuronide	No	Xenobiotics	Drug
_4_acetaminophen_sulfate	No	Xenobiotics	Drug
_4_hydroxycoumarin	No	Xenobiotics	Drug
Carboxyibuprofen	No	Xenobiotics	Drug
Cimetidine	No	Xenobiotics	Drug
Codeine	No	Xenobiotics	Drug
Desmethylnaproxen	No	Xenobiotics	Drug
Desmethylnaproxen_sulfate	No	Xenobiotics	Drug
Doxycycline	No	Xenobiotics	Drug
Gemfibrozil	No	Xenobiotics	Drug
Hydrochlorothiazide	No	Xenobiotics	Drug
Hydroxyibuprofen	No	Xenobiotics	Drug
Ibuprofen	No	Xenobiotics	Drug
Ibuprofen_acyl_glucuronide	No	Xenobiotics	Drug
Metformin	No	Xenobiotics	Drug
Metoprolol	No	Xenobiotics	Drug
Naproxen	No	Xenobiotics	Drug
Nifedipine	No	Xenobiotics	Drug
Quinine	No	Xenobiotics	Drug
Ranitidine	No	Xenobiotics	Drug
Triamterene	No	Xenobiotics	Drug
Verapamil	No	Xenobiotics	Drug
_2_oxindole_3_acetate	No	Xenobiotics	Food component/plant
_3_4_dimethoxycinnamic_acid	No	Xenobiotics	Food component/plant
_3_5_dihydroxybenzoic_acid	No	Xenobiotics	Food component/plant
_3_hydroxycinnamate_sulfate	No	Xenobiotics	Food component/plant
_4_allylphenol_sulfate	No	Xenobiotics	Food component/plant
_4_vinylguaiacol_sulfate	No	Xenobiotics	Food component/plant
Alliin	No	Xenobiotics	Food component/plant
Betonicine	No	Xenobiotics	Food component/plant
Eugenol_sulfate	No	Xenobiotics	Food component/plant

Ferulic_acid_4_sulfate	No	Xenobiotics	Food component/plant
Glycyrrhetinate	No	Xenobiotics	Food component/plant
Indoleacrylate	No	Xenobiotics	Food component/plant
Indolin_2_one	No	Xenobiotics	Food component/plant
Isoeugenol_sulfate	No	Xenobiotics	Food component/plant
Methyl_glucopyranoside__a_b_	No	Xenobiotics	Food component/plant
N_acetylalliin	No	Xenobiotics	Food component/plant
Phytanate	No	Xenobiotics	Food component/plant
Pyrraline	No	Xenobiotics	Food component/plant
S_allylcysteine	No	Xenobiotics	Food component/plant
Sorbate	No	Xenobiotics	Food component/plant
Tartarate	No	Xenobiotics	Food component/plant
Theanine	No	Xenobiotics	Food component/plant
Umbelliferone_sulfate	No	Xenobiotics	Food component/plant
_3_methylurate	No	Xenobiotics	Xanthine metabolism
_7_methylurate	No	Xenobiotics	Xanthine metabolism
Theobromine	No	Xenobiotics	Xanthine metabolism
Citraconate	No	Xenobiotics; energy	Food component/plant; krebs cycle, dicarboxylic acid

Web Table 2. Pathway Analysis for Chemical Class of Metabolites for All-Cause Mortality in the ATBC Study (1985-2013). [a]

Chemical class	No. of contributing metabolites	*P* value
Amino acids [b]	99	0.0016
Nucleotides	20	0.0025
Lipids	152	0.0047
Carbohydrates	19	0.0053
Xenobiotics	56	0.0073
Peptides	23	0.063
Energy	7	0.11
Cofactors and Vitamins	19	0.24

[a] We assessed the associations between chemical classes of metabolites and all-cause mortality using Fisher's method combining *P*-values. We tested a single *P* value for each pathway using parametric bootstrap. For each bootstrap replication, we re-calculated *P*-values from generated vector of score test statistics from multivariate normal distribution with mean 0 and estimated covariance matrix. Pathway *P* values are based on 100,000 permutations.

[b] Below the Bonferroni corrected threshold of $P<0.0021$ (8 tests and 3 outcomes).

Web Table 3. Pathway Analysis for Chemical Sub-Class of Metabolites for All-Cause Mortality in the ATBC Study (1985-2013). [a]

Chemical sub-class	**No. of contributing metabolites**	***P* value**
Primary bile acid metabolism [b]	5	0.00031
Fructose, mannose, galactose, starch, and sucrose metabolism	3	0.00076
Phenylalanine & tyrosine metabolism	16	0.0012
Benzoate metabolism	14	0.0018
Tobacco metabolism	4	0.0019
Glycine, serine and threonine metabolism	8	0.0027
Purine metabolism, guanine containing	4	0.0028
Tryptophan metabolism	12	0.0030
Cysteine, methionine, sam, taurine metabolism	8	0.0059
Long chain fatty acid; polyunsaturated fatty acid (N3 and N6)	6	0.0063
Valine, leucine and Isoleucine metabolism	19	0.012
Long chain fatty acid	12	0.015
Purine metabolism, adenine containing	4	0.018
Secondary bile acid metabolism	9	0.021
Carnitine metabolism	12	0.023
Alanine and aspartate metabolism; pyrimidine metabolism, Uracil containing	3	0.024
Fatty acid metabolism (also bcaa metabolism)	3	0.024
Medium chain fatty acid	8	0.029
Sterol/steroid	22	0.040
Glycerolipid metabolism; phospholipid metabolism	3	0.058
Dipeptide	8	0.061
Pentose metabolism	9	0.066
Lysine metabolism	4	0.078
Purine metabolism, (Hypo)xanthine/Inosine containing	3	0.08
Krebs cycle / TCA cycle	6	0.081
Fatty acid, dicarboxylate	9	0.082
Nicotinate and nicotinamide metabolism	3	0.11
Urea cycle; arginine and proline metabolism	10	0.11
Pyrimidine metabolism, uracil containing	4	0.12
Fatty acid, monohydroxy	7	0.14
Lysolipid	20	0.16
Tocopherol metabolism	5	0.18
Xanthine metabolism	14	0.18
Essential fatty acid; polyunsaturated fatty acid (N3 and N6)	7	0.19
Alanine and aspartate metabolism	4	0.21
Food component/plant	11	0.21

Inositol metabolism	3	0.21
Glycolysis, gluconeogenesis, pyruvate metabolism	5	0.23
Drug	8	0.28
Hemoglobin and porphyrin metabolism	5	0.29
Histidine metabolism	6	0.30
Glutamate metabolism	3	0.35
Gamma-glutamyl amino acid	11	0.41
Monoacylglycerol	10	0.42
Sphingolipid metabolism	4	0.62
Ascorbate and aldarate metabolism	3	0.73

[a] We assessed the associations between chemical subclasses of metabolites and all-cause mortality using Fisher's method combining *P*-values. We tested a single *P* value for each pathway using parametric bootstrap. For each bootstrap replication, we re-calculated *P*-values from generated vector of score test statistics from multivariate normal distribution with mean 0 and estimated covariance matrix. Pathway *P* values are based on 100,000 permutations.

[b] Below the Bonferroni corrected threshold of $P<0.00036$ (46 tests and 3 outcomes).

Web Table 4. Pathway Analysis for Chemical Class of Metabolites for CVD Mortality in the ATBC Study (1985-2013). [a]

Chemical class	No. of contributing metabolites	*P* value
Amino acids [b]	99	0.0019
Nucleotides	20	0.0056
Lipids	152	0.009
Carbohydrates	19	0.015
Peptides	23	0.02
Energy	7	0.044
Cofactors and Vitamins	19	0.063
Xenobiotics	56	0.15

Abbreviations: CVD, cardiovascular disease

[a] We assessed the associations between chemical classes of metabolites and CVD mortality using Fisher's method combining *P*-values. We tested a single *P* value for each pathway using parametric bootstrap. For each bootstrap replication, we re-calculated *P*-values from generated vector of score test statistics from multivariate normal distribution with mean 0 and estimated covariance matrix. Pathway *P* values are based on 100,000 permutations.

[b] Below the Bonferroni corrected threshold of $P<0.0021$ (8 tests and 3 outcomes).

Web Table 5. Pathway Analysis for Chemical Sub-Class of Metabolites for CVD Mortality in the ATBC Study (1985-2013). [a]

Chemical sub-class	**No. of contributing metabolites**	***P* value**
Primary bile acid metabolism [b]	5	0.00027
Phenylalanine & tyrosine metabolism	16	0.00041
Fructose, mannose, galactose, starch, and sucrose metabolism	3	0.0024
Tryptophan metabolism	12	0.0029
Valine, leucine and Isoleucine metabolism	19	0.0047
Purine metabolism, guanine containing	4	0.007
Glycine, serine and threonine metabolism	8	0.010
Sterol/steroid	22	0.015
Secondary bile acid metabolism	9	0.017
Fatty acid metabolism (also bcaa metabolism)	3	0.018
Cysteine, methionine, sam, taurine metabolism	8	0.019
Tocopherol metabolism	5	0.021
Krebs cycle / TCA cycle	6	0.027
Dipeptide	8	0.037
Long chain fatty acid; polyunsaturated fatty acid (N3 and N6)	6	0.037
Lysolipid	20	0.041
Long chain fatty acid	12	0.042
Purine metabolism, adenine containing	4	0.048
Tobacco metabolism	4	0.052
Lysine metabolism	4	0.053
Benzoate metabolism	14	0.058
Carnitine metabolism	12	0.066
Purine metabolism, (Hypo)xanthine/Inosine containing	3	0.074
Fatty acid, dicarboxylate	9	0.075
Pyrimidine metabolism, uracil containing	4	0.085
Medium chain fatty acid	8	0.098
Alanine and aspartate metabolism; pyrimidine metabolism, Uracil containing	3	0.11
Hemoglobin and porphyrin metabolism	5	0.11
Fatty acid, monohydroxy	7	0.12
Essential fatty acid; polyunsaturated fatty acid (N3 and N6)	7	0.14
Glycerolipid metabolism; phospholipid metabolism	3	0.15
Glycolysis, gluconeogenesis, pyruvate metabolism	5	0.15
Inositol metabolism	3	0.17
Alanine and aspartate metabolism	4	0.18
Urea cycle; arginine and proline metabolism	10	0.19
Food component/plant	11	0.21
Pentose metabolism	9	0.23

Gamma-glutamyl amino acid	11	0.26
Histidine metabolism	6	0.28
Ascorbate and aldarate metabolism	3	0.43
Monoacylglycerol	10	0.48
Drug	8	0.53
Xanthine metabolism	14	0.65
Nicotinate and nicotinamide metabolism	3	0.72
Glutamate metabolism	3	0.77
Sphingolipid metabolism	4	0.89

Abbreviations: CVD, cardiovascular disease

[a] We assessed the associations between chemical subclasses of metabolites and CVD mortality using Fisher's method combining *P*-values. We tested a single *P* value for each pathway using parametric bootstrap. For each bootstrap replication, we re-calculated *P*-values from generated vector of score test statistics from multivariate normal distribution with mean 0 and estimated covariance matrix. Pathway *P* values are based on 100,000 permutations.

[b] Below the Bonferroni corrected threshold of $P<0.00036$ (46 tests and 3 outcomes).

Web Table 6. Pathway Analysis for Chemical Class of Metabolites for Cancer Mortality in the ATBC Study (1985-2013). [a]

Chemical class	**No. of contributing metabolites**	***P* value**
Xenobiotics	56	0.023
Amino acids	99	0.034
Nucleotides	20	0.051
Lipids	152	0.13
Peptides	23	0.18
Carbohydrates	19	0.47
Cofactors and Vitamins	19	0.77
Energy	7	0.82

[a] We assessed the associations between chemical classes of metabolites and cancer mortality using Fisher's method combining *P*-values. We tested a single *P* value for each pathway using parametric bootstrap. For each bootstrap replication, we re-calculated *P*-values from generated vector of score test statistics from multivariate normal distribution with mean 0 and estimated covariance matrix. Pathway *P* values are based on 100,000 permutations.

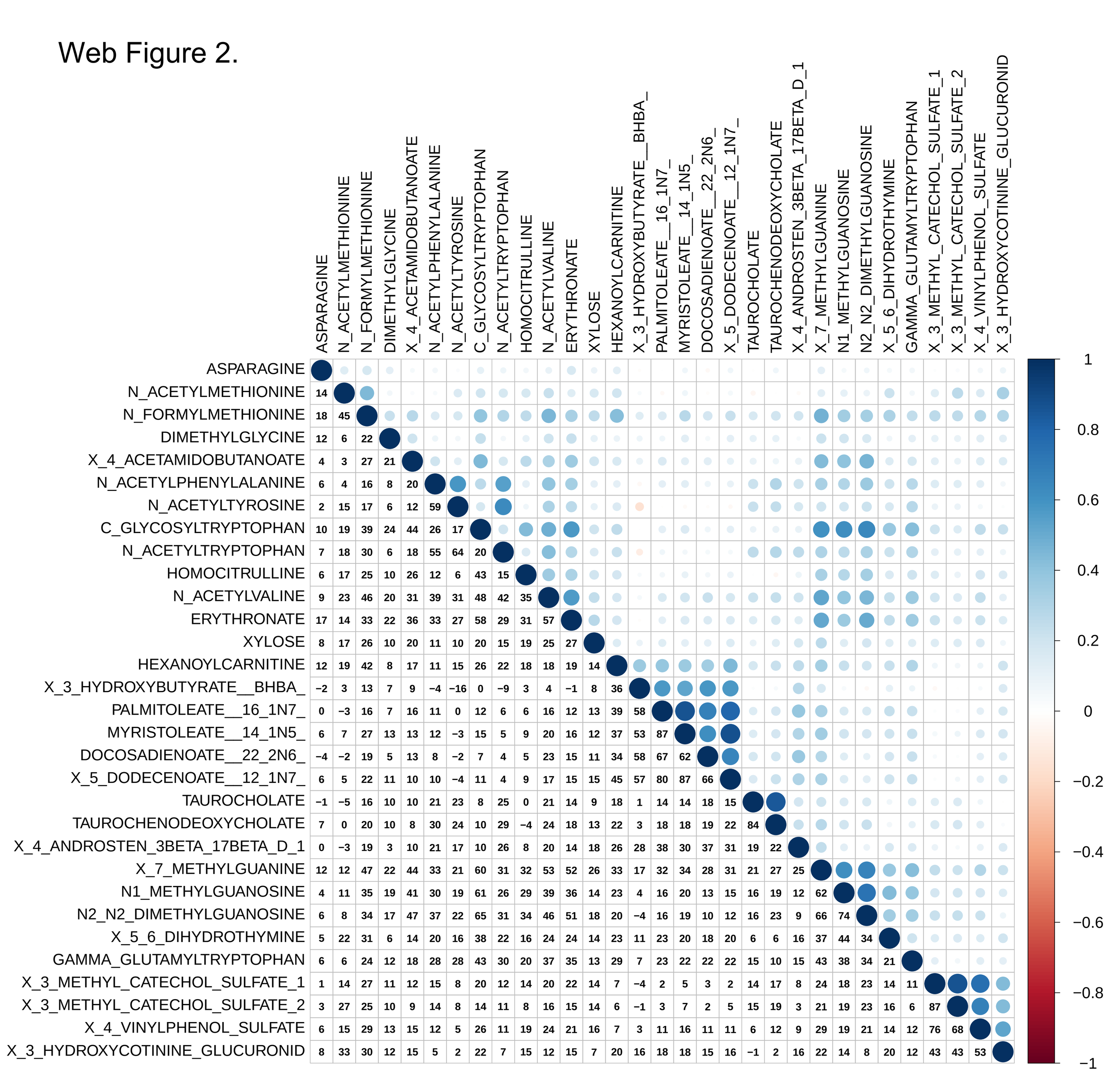
Web Table 7. Pathway Analysis for Chemical Sub-Class of Metabolites for Cancer Mortality in the ATBC Study (1985-2013). [a]

Chemical sub-class	**No. of contributing metabolites**	***P* value**
Tobacco metabolism	4	0.0030
Benzoate metabolism	14	0.0036
Phenylalanine & tyrosine metabolism	16	0.0078
Tryptophan metabolism	12	0.013
Glycine, serine and threonine metabolism	8	0.030
Purine metabolism, guanine containing	4	0.035
Dipeptide	8	0.036
Cysteine, methionine, sam, taurine metabolism	8	0.039
Food component/plant	11	0.052
Fructose, mannose, galactose, starch, and sucrose metabolism	3	0.069
Valine, leucine and Isoleucine metabolism	19	0.089
Secondary bile acid metabolism	9	0.092
Purine metabolism, adenine containing	4	0.12
Carnitine metabolism	12	0.13
Fatty acid metabolism (also BCAA metabolism)	3	0.14
Medium chain fatty acid	8	0.14
Glycerolipid metabolism; phospholipid metabolism	3	0.16
Long chain fatty acid	12	0.16
Sterol/steroid	22	0.17
Long chain fatty acid; polyunsaturated fatty acid (N3 and N6)	6	0.21
Drug	8	0.22
Fatty acid, dicarboxylate	9	0.24
Pyrimidine metabolism, uracil containing	4	0.26
Fatty acid, monohydroxy	7	0.27
Nicotinate and nicotinamide metabolism	3	0.28
Urea cycle; arginine and proline metabolism	10	0.31
Inositol metabolism	3	0.32
Histidine metabolism	6	0.35
Monoacylglycerol	10	0.36
Primary bile acid metabolism	5	0.38
Hemoglobin and porphyrin metabolism	5	0.40
Purine metabolism, (Hypo)xanthine/Inosine containing	3	0.46
Lysolipid	20	0.50
Xanthine metabolism	14	0.50
Alanine and aspartate metabolism; pyrimidine metabolism, Uracil containing	3	0.55
Pentose metabolism	9	0.67

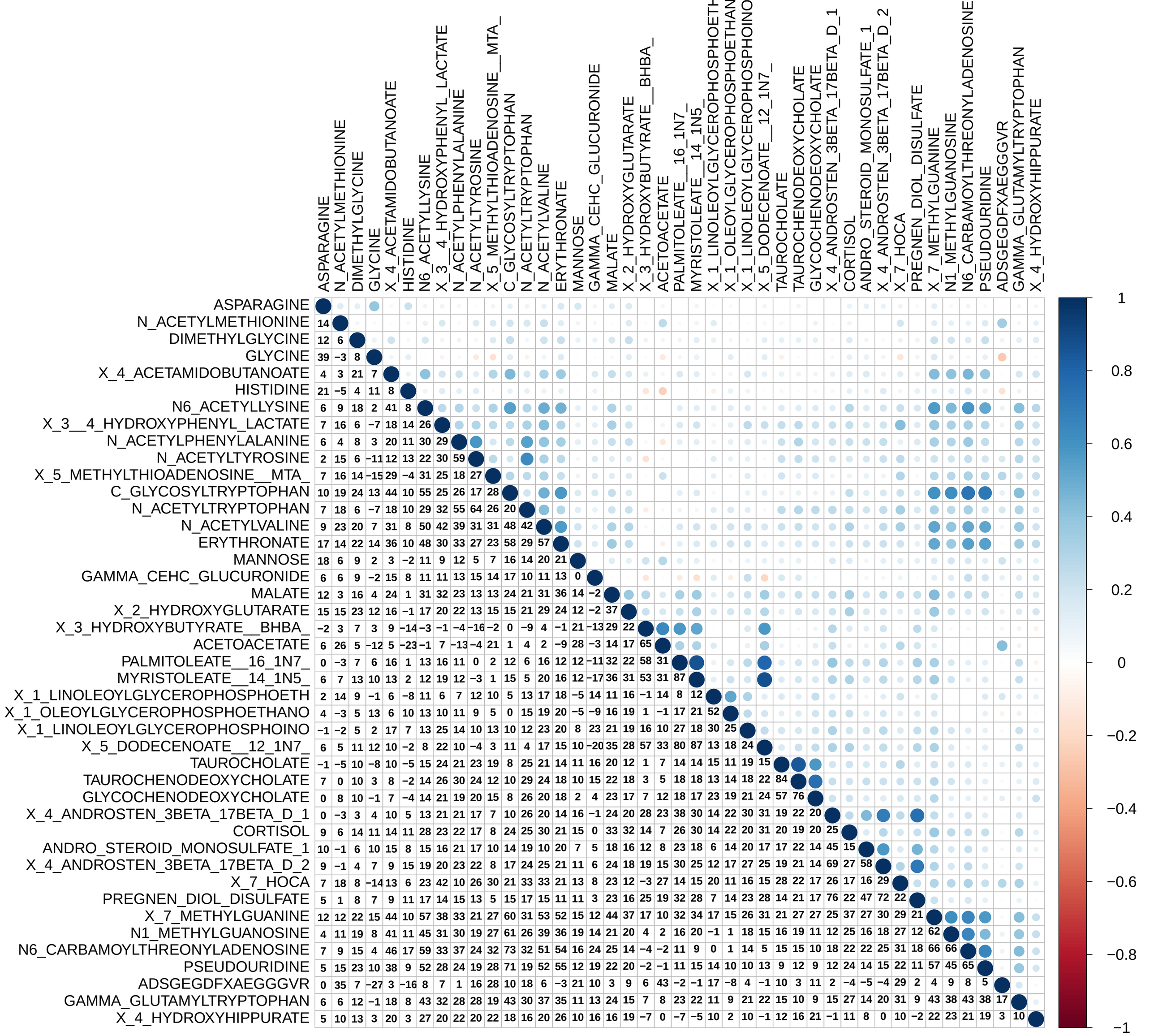
Essential fatty acid; polyunsaturated fatty acid (N3 and N6)	7	0.72
Glutamate metabolism	3	0.73
Alanine and aspartate metabolism	4	0.73
Tocopherol metabolism	5	0.74
Krebs cycle / TCA cycle	6	0.76
Gamma-glutamyl amino acid	11	0.79
Ascorbate and aldarate metabolism	3	0.81
Sphingolipid metabolism	4	0.95
Glycolysis, gluconeogenesis, pyruvate metabolism	5	0.95
Lysine metabolism	4	0.96

[a] We assessed the associations between chemical subclasses of metabolites and cancer mortality using Fisher's method combining *P*-values. We tested a single *P* value for each pathway using parametric bootstrap. For each bootstrap replication, we re-calculated *P*-values from generated vector of score test statistics from multivariate normal distribution with mean 0 and estimated covariance matrix. Pathway *P* values are based on 100,000 permutations.

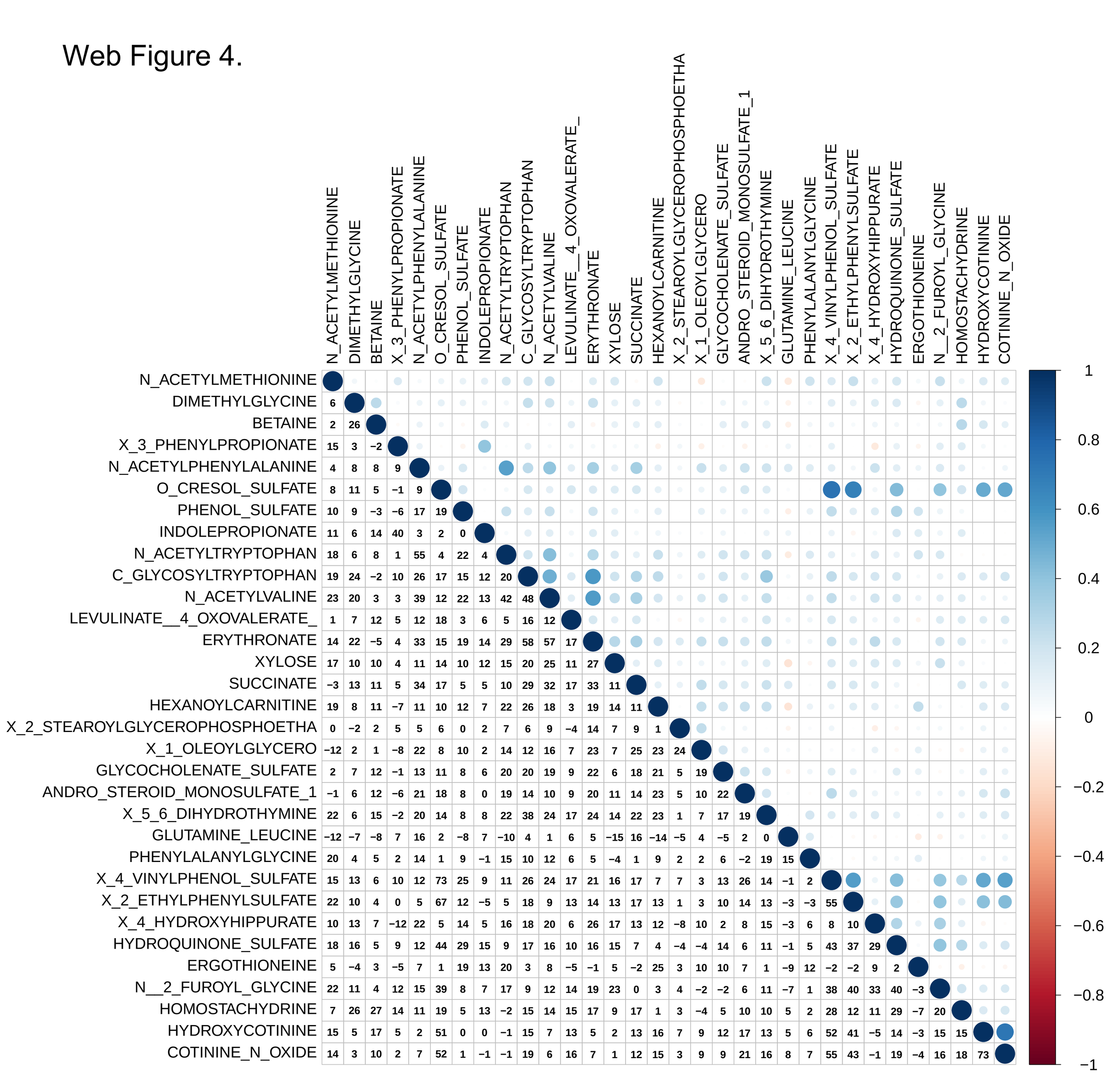
Web Figure 2.


ASPARAGINE
N_ACETYLMETHIONINE
N_FORMYLMETHIONINE
DIMETHYLGLYCINE
X_4_ACETAMIDOBUTANOATE
N_ACETYLPHENYLALANINE
N_ACETYLTYROSINE
C_GLYCOSYLTRYPTOPHAN
N_ACETYLTRYPTOPHAN
HOMOCITRULLINE
N_ACETYLVALINE
ERYTHRONATE
XYLOSE
HEXANOYLCARNITINE
X_3_HYDROXYBUTYRATE__BHBA_
PALMITOLEATE__16_1N7_
MYRISTOLEATE__14_1N5_
DOCOSADIENOATE__22_2N6_
X_5_DODECENOATE__12_1N7_
TAUROCHOLATE
TAUROCHENODEOXYCHOLATE
X_4_ANDROSTEN_3BETA_17BETA_D_1
X_7_METHYLGUANINE
N1_METHYLGUANOSINE
N2_N2_DIMETHYLGUANOSINE
X_5_6_DIHYDROTHYMINE
GAMMA_GLUTAMYLTRYPTOPHAN
X_3_METHYL_CATECHOL_SULFATE_1
X_3_METHYL_CATECHOL_SULFATE_2
X_4_VINYLPHENOL_SULFATE
X_3_HYDROXYCOTININE_GLUCURONID
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1

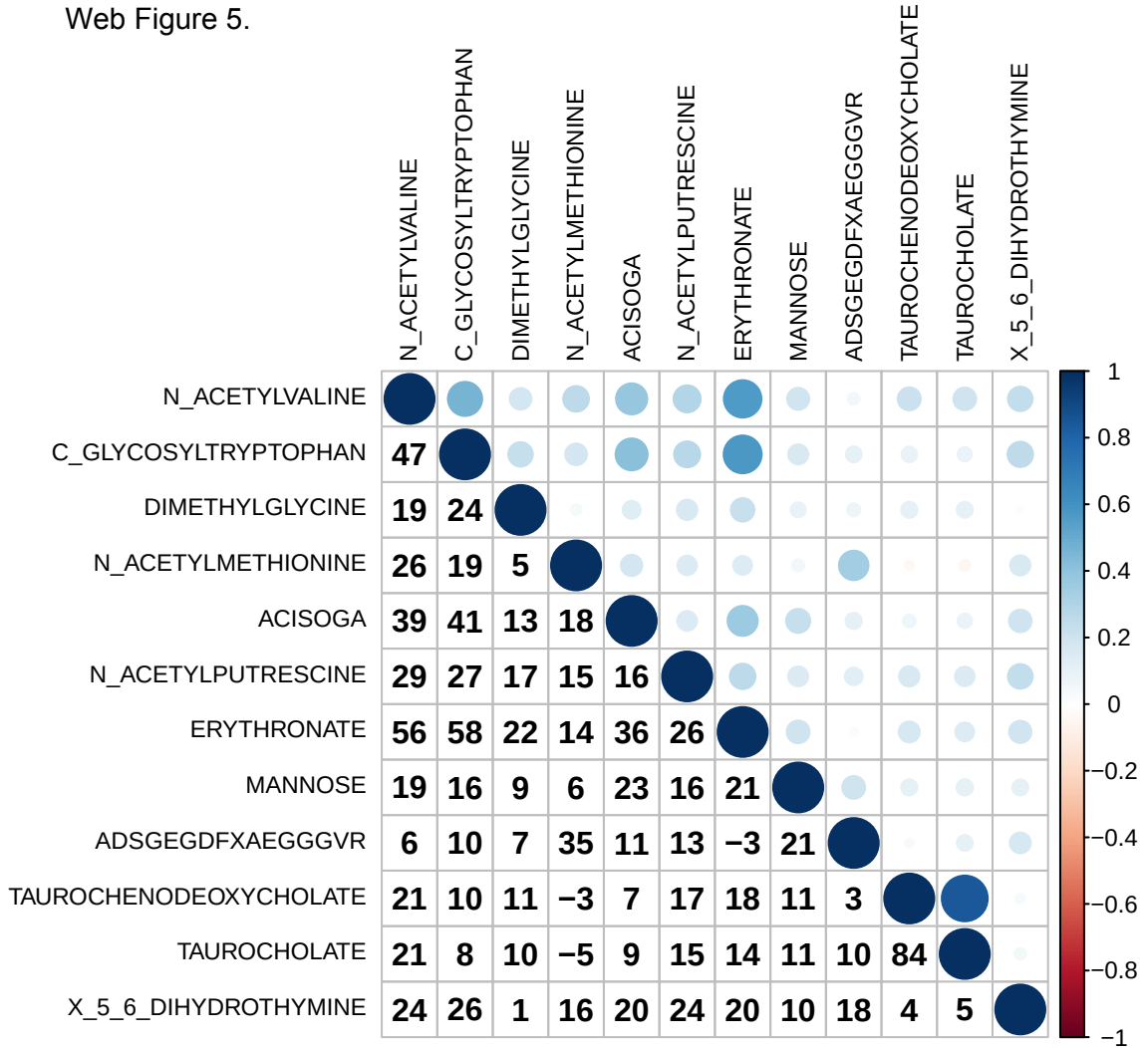
Web Figure 3.


ASPARAGINE
N_ACETYLMETHIONINE
DIMETHYLGLYCINE
GLYCINE
X_4_ACETAMIDOBUTANOATE
HISTIDINE
N6_ACETYLLYSINE
X_3__4_HYDROXYPHENYL_LACTATE
N_ACETYLPHENYLALANINE
N_ACETYLTYROSINE
X_5_METHYLTHIOADENOSINE__MTA_
C_GLYCOSYLTRYPTOPHAN
N_ACETYLTRYPTOPHAN
N_ACETYLVALINE
ERYTHRONATE
MANNOSE
GAMMA_CEHC_GLUCURONIDE
MALATE
X_2_HYDROXYGLUTARATE
X_3_HYDROXYBUTYRATE__BHBA_
ACETOACETATE
PALMITOLEATE__16_1N7_
MYRISTOLEATE__14_1N5_
X_1_LINOLEOYLGLYCEROPHOSPHOETH
X_1_OLEOYLGLYCEROPHOSPHOETHANO
X_1_LINOLEOYLGLYCEROPHOSPHOINO
X_5_DODECENOATE__12_1N7_
TAUROCHOLATE
TAUROCHENODEOXYCHOLATE
GLYCOCHENODEOXYCHOLATE
X_4_ANDROSTEN_3BETA_17BETA_D_1
CORTISOL
ANDRO_STEROID_MONOSULFATE_1
X_4_ANDROSTEN_3BETA_17BETA_D_2
X_7_HOCA
PREGNEN_DIOL_DISULFATE
X_7_METHYLGUANINE
N1_METHYLGUANOSINE
N6_CARBAMOYLTHREONYLADENOSINE
PSEUDOURIDINE
ADSGEGDFXAEGGGVR
GAMMA_GLUTAMYLTRYPTOPHAN
X_4_HYDROXYHIPPURATE
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1

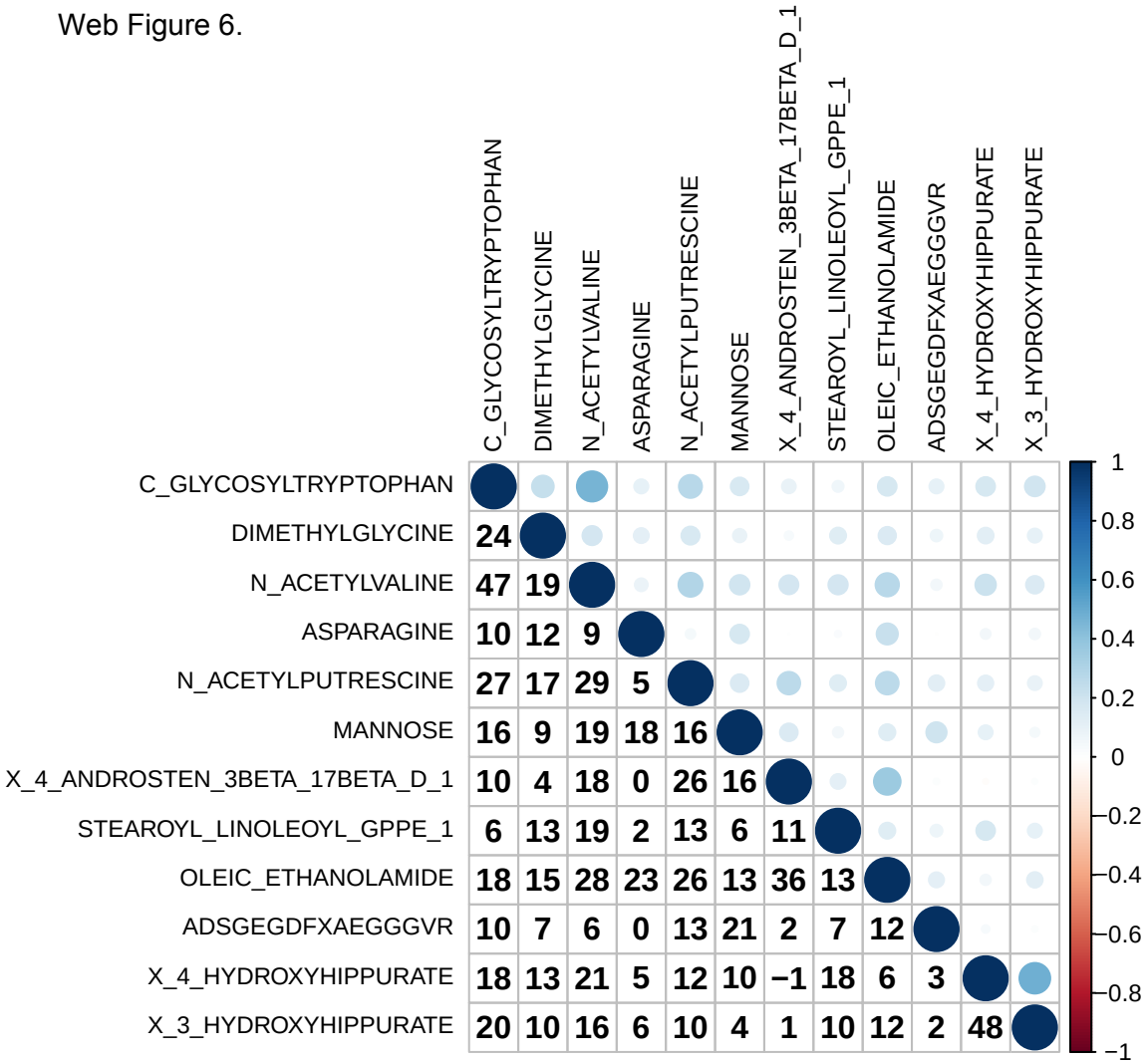
Web Figure 4.


N_ACETYLMETHIONINE
DIMETHYLGLYCINE
BETAINE
X_3_PHENYLPROPIONATE
N_ACETYLPHENYLALANINE
O_CRESOL_SULFATE
PHENOL_SULFATE
INDOLEPROPIONATE
N_ACETYLTRYPTOPHAN
C_GLYCOSYLTRYPTOPHAN
N_ACETYLVALINE
LEVULINATE__4_OXOVALERATE_
ERYTHRONATE
XYLOSE
SUCCINATE
HEXANOYLCARNITINE
X_2_STEAROYLGLYCEROPHOSPHOETHA
X_1_OLEOYLGLYCERO
GLYCOCHOLENATE_SULFATE
ANDRO_STEROID_MONOSULFATE_1
X_5_6_DIHYDROTHYMINE
GLUTAMINE_LEUCINE
PHENYLALANYLGLYCINE
X_4_VINYLPHENOL_SULFATE
X_2_ETHYLPHENYLSULFATE
X_4_HYDROXYHIPPURATE
HYDROQUINONE_SULFATE
ERGOTHIONEINE
N__2_FUROYL_GLYCINE
HOMOSTACHYDRINE
HYDROXYCOTININE
COTININE_N_OXIDE
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1

Web Figure 5.


N_ACETYLVALINE
C_GLYCOSYLTRYPTOPHAN
DIMETHYLGLYCINE
N_ACETYLMETHIONINE
ACISOGA
N_ACETYLPUTRESCINE
ERYTHRONATE
MANNOSE
ADSGEGDFXAEGGGVR
TAUROCHENODEOXYCHOLATE
TAUROCHOLATE
X_5_6_DIHYDROTHYMINE
N_ACETYLVALINE
C_GLYCOSYLTRYPTOPHAN 47
DIMETHYLGLYCINE 19 24
N_ACETYLMETHIONINE 26 19 5
ACISOGA 39 41 13 18
N_ACETYLPUTRESCINE 29 27 17 15 16
ERYTHRONATE 56 58 22 14 36 26
MANNOSE 19 16 9 6 23 16 21
ADSGEGDFXAEGGGVR 6 10 7 35 11 13 −3 21
TAUROCHENODEOXYCHOLATE 21 10 11 −3 7 17 18 11 3
TAUROCHOLATE 21 8 10 −5 9 15 14 11 10 84
X_5_6_DIHYDROTHYMINE 24 26 1 16 20 24 20 10 18 4 5
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1

Web Figure 6.


C_GLYCOSYLTRYPTOPHAN
DIMETHYLGLYCINE
N_ACETYLVALINE
ASPARAGINE
N_ACETYLPUTRESCINE
MANNOSE
X_4_ANDROSTEN_3BETA_17BETA_D_1
STEAROYL_LINOLEOYL_GPPE_1
OLEIC_ETHANOLAMIDE
ADSGEGDFXAEGGGVR
X_4_HYDROXYHIPPURATE
X_3_HYDROXYHIPPURATE
C_GLYCOSYLTRYPTOPHAN
DIMETHYLGLYCINE 24
N_ACETYLVALINE 47 19
ASPARAGINE 10 12 9
N_ACETYLPUTRESCINE 27 17 29 5
MANNOSE 16 9 19 18 16
X_4_ANDROSTEN_3BETA_17BETA_D_1 10 4 18 0 26 16
STEAROYL_LINOLEOYL_GPPE_1 6 13 19 2 13 6 11
OLEIC_ETHANOLAMIDE 18 15 28 23 26 13 36 13
ADSGEGDFXAEGGGVR 10 7 6 0 13 21 2 7 12
X_4_HYDROXYHIPPURATE 18 13 21 5 12 10 −1 18 6 3
X_3_HYDROXYHIPPURATE 20 10 16 6 10 4 1 10 12 2 48
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1