

# **SUPPLEMENTAL MATERIAL**

## **DATA S1: SUPPLEMENTAL METHODS**

### *Quality Assurance and Control*

Several types of controls were analyzed in concert with the experimental samples. Specifically, a pooled matrix sample generated by taking a small volume of each experimental sample served as a technical replicate throughout the data set. Extracted water samples served as process blanks and a cocktail of quality control (QC) standards chosen not to interfere with the measurement of endogenous compounds were spiked into every analyzed sample to allow for instrument performance monitoring and aided chromatographic alignment. Instrument variability was determined by calculating the median relative standard deviation (RSD) for the standards that were added to each sample prior to injection into the mass spectrometers. Process variability was determined by calculating the median RSD for all endogenous metabolites (*i.e.*, non-instrument standards) present in 100% of the pooled matrix samples. Experimental samples were randomized across the platform run with QC samples spaced evenly among the injections.

**Table S1: TTE vs no TTE**

	<b>No TTE (N=98)</b>	<b>TTE (N=89)</b>	<b>p-value</b>
<b>Age (mean, SD)</b>	50.0 (11.4)	50.4 (9.4)	0.77
<b>Female (n, %)</b>	61 (62.2)	38 (42.7)	0.01
<b>Race (n, %)</b>			0.56
<b>White</b>	84 (85.7)	82 (92.1)	
<b>Black</b>	8 (8.2)	4 (4.5)	
<b>BMI (mean, SD)</b>	34.2 (7.3)	36.4 (7.0)	0.04
<b>Diabetes mellitus (%)</b>	35 (35.7)	32 (36.0)	1
<b>Hemoglobin A1c (mean, SD)</b>	6.1 (0.9)	6.6 (1.6)	0.03
<b>Hypertension</b>	54 (55.1)	67 (75.3)	0.006
<b>Total cholesterol (mean, SD)</b>	201.0 (56.2)	184.2 (44.9)	0.04
<b>LDL (mean, SD)</b>	120.0 (34.6)	111.3 (39.0)	0.15
<b>HDL (mean, SD)</b>	42.47 (14.6)	37.84 (13.7)	0.04
<b>Hyperlipidemia</b>	36 (36.7)	37 (41.6)	0.60
<b>Hypertriglyceridemia</b>	18 (18.4)	12 (13.5)	0.48
<b>AST (mean, SD)</b>	70.5 (53.9)	64.5 (42.9)	0.41
<b>ALT (mean, SD)</b>	93.9 (73.2)	80.3 (50.3)	0.15
<b>Fibrosis stage (n, %)</b>			0.07
<b>Stage 0</b>	9 (9.2)	3 (3.4)	
<b>Stage 1</b>	20 (20.4)	16 (18.0)	
<b>Stage 2</b>	51 (52.0)	39 (43.8)	
<b>Stage 3</b>	14 (14.3)	27 (30.3)	
<b>Stage 4</b>	4 (4.1)	4 (4.5)	
<b>NASH Activity Score</b>			0.72
<b>1</b>	2 (2.2)	1 (1.2)	
<b>2</b>	11 (12.1)	6 (7.1)	
<b>3</b>	14 (15.4)	12 (14.1)	
<b>4</b>	19 (20.9)	27 (31.8)	
<b>5</b>	23 (25.3)	20 (23.5)	
<b>6</b>	13 (14.3)	12 (14.1)	
<b>7</b>	9 (9.9)	7 (8.2)	

TTE = transthoracic echocardiogram; SD = standard deviation; LDL = low-density lipoprotein; HDL = high-density lipoprotein; AST = aspartate aminotransferase; ALT = alanine aminotransferase; NASH = non-alcoholic steatohepatitis

**Table S2: Missing metabolite values by HFpEF definition\***

	HFpEF		HFpEF No Fatigue		Diastolic dysfunction	
	No	Yes	No	Yes	No	Yes
Missing values (%, IQR)	2.4% (1.8-3.2)	2.6% (1.8-3.0)	2.4% (1.8-3.2)	2.6% (1.8-2.7)	2.4% (1.8-3.3)	2.4% (1.8-3.0)

\*For entire cohort of 89 patients: 2.4% (IQR: 1.8-3.0)

HFpEF = heart failure with preserved ejection fraction; IQR = interquartile range

**Table S3: HFpEF full results\***

Metabolite	Pathway	Sub-Pathway	log Fold change	Unadjusted p-value	Adjusted p-value
1-arachidonoyl-GPE* (20:4)*	Lipid	Lysolipid	0.28	0.0001	0.06
1-docosahexaenoylglycerophosphoethanolamine*	Lipid	Lysolipid	0.37	0.0003	0.10
2-stearoylglycerophosphoethanolamine*	Lipid	Lysolipid	0.33	0.001	0.16
1-stearoyl-GPE (18:0)	Lipid	Lysolipid	0.26	0.002	0.19
2-arachidonoyl-GPE* (20:4)*	Lipid	Lysolipid	0.58	0.002	0.19
1-arachidonoyl-GPC* (20:4)*	Lipid	Lysolipid	0.27	0.002	0.19
azelate (nonanedioate; C9)	Lipid	Fatty Acid, Dicarboxylate	-0.31	0.003	0.19
2-arachidonoyl-GPC* (20:4)*	Lipid	Lysolipid	0.32	0.003	0.19
alpha-ketoglutarate	Energy	TCA Cycle	0.32	0.003	0.19
1-palmitoyl-GPC (16:0)	Lipid	Lysolipid	0.23	0.003	0.19
TL18:3n6 (g-linolenic acid)	Lipid	Mole % Total Fatty Acid	0.24	0.004	0.19
1-myristoyl-GPC (14:0)	Lipid	Lysolipid	0.40	0.004	0.19
1-oleoyl-GPE (18:1)	Lipid	Lysolipid	0.24	0.004	0.19
2-oleoyl-GPE* (18:1)*	Lipid	Lysolipid	0.85	0.004	0.19
2-palmitoleoyl-GPC* (16:1)*	Lipid	Lysolipid	0.53	0.005	0.19
1-palmitoyl-GPE (16:0)	Lipid	Lysolipid	0.24	0.005	0.19
palmitoyl-arachidonoylglycerophosphocholine (2)*	Lipid	Lysolipid	0.17	0.005	0.19
2-hydroxy-3-methylvalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.27	0.006	0.19
2-myristoyl-GPC* (14:0)*	Lipid	Lysolipid	0.55	0.006	0.19
1-oleoyl-GPC (18:1)	Lipid	Lysolipid	0.28	0.006	0.19
1-arachidonoylglycerol	Lipid	Monoacylglycerol	0.24	0.006	0.20
1-linolenoylglycerophosphocholine (18:3n3)*	Lipid	Lysolipid	0.34	0.007	0.20
citrate	Energy	TCA Cycle	-0.18	0.008	0.21
cysteine s-sulfate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.20	0.008	0.21
2-docosahexaenoyl-GPC* (22:6)*	Lipid	Lysolipid	0.40	0.008	0.21
caproate (6:0)	Lipid	Medium Chain Fatty Acid	-0.16	0.009	0.22
2-palmitoyl-GPC* (16:0)*	Lipid	Lysolipid	0.25	0.009	0.22
1-eicosapentaenoylglycerophosphocholine (20:5n3)*	Lipid	Lysolipid	0.47	0.009	0.22
1-stearoyl-GPC (18:0)	Lipid	Lysolipid	0.29	0.01	0.23

<b>glucose</b>	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.14	0.01	0.25
<b>2-palmitoyl-GPE* (16:0)*</b>	Lipid	Lysolipid	0.28	0.01	0.25
<b>1-palmitoleoyl-GPC* (16:1)*</b>	Lipid	Lysolipid	0.32	0.01	0.25
<b>N6-acetyllysine</b>	Amino Acid	Lysine Metabolism	0.12	0.01	0.27
<b>1-pentadecanoylglycerophosphocholine (15:0)*</b>	Lipid	Lysolipid	0.25	0.01	0.27
<b>methyl glucopyranoside (alpha + beta)</b>	Xenobiotics	Food Component/Plant	-0.72	0.02	0.29
<b>1-docosahexaenoyl-GPC* (22:6)*</b>	Lipid	Lysolipid	0.28	0.02	0.29
<b>2-eicosatrienoyl-GPC* (20:3)*</b>	Lipid	Lysolipid	0.21	0.02	0.32
<b>1-docosahexaenoylglycerol</b>	Lipid	Monoacylglycerol	0.32	0.02	0.32
<b>1-eicosatrienoylglycerophosphoethanolamine*</b>	Lipid	Lysolipid	0.55	0.02	0.35
<b>1-eicosatrienoyl-GPC* (20:3)*</b>	Lipid	Lysolipid	0.23	0.02	0.35
<b>1-docosapentaenoyl-GPC* (22:5n3)*</b>	Lipid	Lysolipid	0.26	0.02	0.35
<b>ribitol</b>	Carbohydrate	Pentose Metabolism	0.14	0.02	0.38
<b>propionylglycine (C3)</b>	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.26	0.03	0.40
<b>phenylpyruvate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.17	0.03	0.40
<b>1-linolenoylglycerol</b>	Lipid	Monoacylglycerol	0.25	0.03	0.41
<b>N2-methylguanosine</b>	Nucleotide	Purine Metabolism, Guanine containing	0.22	0.03	0.44
<b>2-stearoyl-GPC* (18:0)*</b>	Lipid	Lysolipid	0.29	0.03	0.44
<b>1-palmitoylplasmylethanolamine*</b>	Lipid	Lysolipid	0.17	0.03	0.44
<b>eugenol sulfate</b>	Xenobiotics	Food Component/Plant	0.87	0.03	0.45
<b>N-acetyltryptophan</b>	Amino Acid	Tryptophan Metabolism	0.23	0.04	0.46
<b>2-docosahexaenoylglycerol*</b>	Lipid	Monoacylglycerol	0.69	0.04	0.48
<b>2-hydroxyisobutyrate</b>	Xenobiotics	Chemical	0.20	0.04	0.49
<b>adrenate (22:4n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.18	0.04	0.51
<b>benzoate</b>	Xenobiotics	Benzoate Metabolism	-0.14	0.04	0.53
<b>S-methylcysteine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.20	0.04	0.53
<b>3-methoxytyrosine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.13	0.05	0.53
<b>mannose</b>	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.14	0.05	0.55
<b>methionine sulfone</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.29	0.05	0.57
<b>3b-hydroxy-5-cholenoic acid</b>	Lipid	Secondary Bile Acid Metabolism	-0.48	0.06	0.61

<b>1-stearoylplasménylethanolamine*</b>	Lipid	Lysolipid	0.22	0.06	0.61
<b>3-methyl-2-oxobutyrate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.11	0.06	0.61
<b>N6-succinyladenosine</b>	Nucleotide	Purine Metabolism, Adenine containing	0.14	0.06	0.61
<b>2-linoleoyl-GPC* (18:2)*</b>	Lipid	Lysolipid	0.19	0.06	0.61
<b>2-arachidonoyl glycerol</b>	Lipid	Monoacylglycerol	0.20	0.06	0.61
<b>1-oleoylplasménylethanolamine*</b>	Lipid	Lysolipid	0.19	0.06	0.61
<b>beta-hydroxyisovalerate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.18	0.06	0.61
<b>malonate (propanedioate)</b>	Lipid	Fatty Acid Synthesis	-0.29	0.06	0.61
<b>7-alpha-hydroxycholesterol</b>	Lipid	Sterol	0.33	0.06	0.61
<b>fucose</b>	Carbohydrate	Pentose Metabolism	0.19	0.07	0.61
<b>2-oleoyl-GPC* (18:1)*</b>	Lipid	Lysolipid	0.17	0.07	0.61
<b>phenylalanyleucine</b>	Peptide	Dipeptide	0.55	0.07	0.61
<b>stearoyl-arachidonoyl-glycerophosphoethanolamine (1)*</b>	Lipid	Lysolipid	0.20	0.07	0.61
<b>cytidine</b>	Nucleotide	Pyrimidine Metabolism, Cytidine containing	0.16	0.07	0.61
<b>docosahexaenoate (DHA; 22:6n3)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.19	0.07	0.61
<b>xylitol</b>	Carbohydrate	Pentose Metabolism	0.28	0.07	0.61
<b>pyruvate</b>	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.26	0.07	0.61
<b>sulfate*</b>	Xenobiotics	Chemical	0.07	0.07	0.61
<b>1-methyladenosine</b>	Nucleotide	Purine Metabolism, Adenine containing	0.09	0.07	0.61
<b>TL20:3n9 (mead acid)</b>	Lipid	Mole % Total Fatty Acid	0.24	0.08	0.61
<b>alpha-hydroxyisovalerate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.21	0.08	0.61
<b>stearidonate (18:4n3)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.23	0.08	0.61
<b>serylleucine</b>	Peptide	Dipeptide	-0.67	0.08	0.61
<b>3-methylglutaconate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.27	0.08	0.61
<b>1-heptadecanoyl-GPC (17:0)</b>	Lipid	Lysolipid	0.32	0.08	0.62
<b>3-hydroxy-3-methylglutarate</b>	Lipid	Mevalonate Metabolism	0.12	0.08	0.64
<b>TL18:4n3 (stearidonic acid)</b>	Lipid	Mole % Total Fatty Acid	0.34	0.09	0.64
<b>1-eicosenoylglycerophosphocholine (20:1n9)*</b>	Lipid	Lysolipid	0.25	0.09	0.64
<b>indoleacetylglutamine</b>	Amino Acid	Tryptophan Metabolism	0.55	0.09	0.65
<b>3-methylglutaryl carnitine (2)</b>	Amino Acid	Lysine Metabolism	0.27	0.09	0.65
<b>2-ethylhexanoic acid</b>	Xenobiotics	Chemical	-0.14	0.09	0.65

<b>hexanoylglycine (C6)</b>	Lipid	Fatty Acid Metabolism(Acyl Glycine)	0.53	0.09	0.65
<b>orotate</b>	Nucleotide	Pyrimidine Metabolism, Orotate containing	0.28	0.09	0.65
<b>1-linoleoyl-GPC (18:2)</b>	Lipid	Lysolipid	0.14	0.09	0.65
<b>betaine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.10	0.10	0.68
<b>N-acetylputrescine</b>	Amino Acid	Polyamine Metabolism	0.16	0.10	0.68
<b>ethylmalonate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.18	0.10	0.68
<b>2-palmitoylglycerol (16:0)</b>	Lipid	Monoacylglycerol	0.26	0.10	0.68
<b>stearylcarntine (C18)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.19	0.10	0.69
<b>glutamine</b>	Amino Acid	Glutamate Metabolism	-0.06	0.11	0.69
<b>1-methylnicotinamide</b>	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-0.43	0.11	0.69
<b>tetradecanedioate (C14)</b>	Lipid	Fatty Acid, Dicarboxylate	-0.21	0.11	0.69
<b>hexadecanedioate (C16)</b>	Lipid	Fatty Acid, Dicarboxylate	-0.20	0.11	0.69
<b>TL20:5n3 (eicosapentaenoic acid)</b>	Lipid	Mole % Total Fatty Acid	0.24	0.11	0.69
<b>eicosapentaenoate (EPA; 20:5n3)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.25	0.11	0.69
<b>1-arachidoyl-GPC (20:0)</b>	Lipid	Lysolipid	0.51	0.11	0.69
<b>stearyl-arachidonoyl-glycerophosphocholine (2)*</b>	Lipid	Lysolipid	0.11	0.11	0.69
<b>3-hydroxyoctanoate</b>	Lipid	Fatty Acid, Monohydroxy	-0.18	0.11	0.70
<b>dimethylarginine (ADMA + SDMA)</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.05	0.12	0.72
<b>sphinganine</b>	Lipid	Sphingolipid Metabolism	0.51	0.12	0.73
<b>arachidonate (20:4n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.09	0.12	0.73
<b>6-oxopiperidine-2-carboxylic acid</b>	Xenobiotics	Drug	0.14	0.12	0.73
<b>TL22:5n3 (docosapentaenoic acid)</b>	Lipid	Mole % Total Fatty Acid	0.11	0.13	0.74
<b>alpha-hydroxycaproate</b>	Lipid	Fatty Acid, Monohydroxy	0.13	0.13	0.74
<b>5,6-dihydrothymine</b>	Nucleotide	Pyrimidine Metabolism, Thymine containing	-0.12	0.13	0.74
<b>3-hydroxy-2-ethylpropionate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.12	0.13	0.74
<b>stearate (18:0)</b>	Lipid	Long Chain Fatty Acid	0.07	0.13	0.74
<b>1-eicosadienoyl-GPC* (20:2)*</b>	Lipid	Lysolipid	0.20	0.13	0.74
<b>3-methyl catechol sulfate (1)</b>	Xenobiotics	Benzoate Metabolism	0.47	0.13	0.74
<b>glutamate</b>	Amino Acid	Glutamate Metabolism	0.12	0.14	0.74
<b>trimethylamine N-oxide</b>	Lipid	Phospholipid Metabolism	0.67	0.14	0.75
<b>dopamine sulfate (2)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.16	0.14	0.75
<b>myristoylcarnitine</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.20	0.14	0.75
<b>phenyllactate (PLA)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.11	0.14	0.75



<b>gamma-glutamylalanine</b>	Peptide	Gamma-glutamyl Amino Acid	0.14	0.14	0.75
<b>2-aminooctanoate</b>	Lipid	Fatty Acid, Amino	0.19	0.14	0.75
<b>N-acetylglycine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	0.18	0.14	0.75
<b>TL20:1n9 (eicosanoic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.07	0.14	0.75
<b>1,2,3-benzenetriol sulfate (2)</b>	Xenobiotics	Chemical	-0.67	0.15	0.75
<b>xanthosine</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.16	0.15	0.75
<b>TL16:1n7 (palmitoleic acid)</b>	Lipid	Mole % Total Fatty Acid	0.14	0.16	0.75
<b>4-hydroxyhippurate</b>	Xenobiotics	Benzoate Metabolism	-0.28	0.16	0.75
<b>2-linoleoyl-GPE* (18:2)*</b>	Lipid	Lysolipid	0.17	0.16	0.75
<b>9,10-DiHOME</b>	Lipid	Fatty Acid, Dihydroxy	-0.30	0.16	0.75
<b>palmitoylcarnitine (C16)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.15	0.16	0.75
<b>TL18:2n6 (linoleic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.07	0.16	0.75
<b>indolepropionate</b>	Amino Acid	Tryptophan Metabolism	-0.28	0.16	0.75
<b>3-ureidopropionate</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.14	0.16	0.75
<b>1-stearoylglycerol (18:0)</b>	Lipid	Monoacylglycerol	0.42	0.16	0.75
<b>N-acetylleucine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.12	0.16	0.75
<b>myristoyl sphingomyelin*</b>	Lipid	Sphingolipid Metabolism	0.07	0.16	0.75
<b>alpha-ketobutyrate</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.29	0.16	0.75
<b>dodecanedioate (C12)</b>	Lipid	Fatty Acid, Dicarboxylate	-0.18	0.17	0.76
<b>cysteine-glutathione disulfide</b>	Amino Acid	Glutathione Metabolism	-0.38	0.17	0.76
<b>4-imidazoleacetate</b>	Amino Acid	Histidine Metabolism	-0.36	0.17	0.76
<b>TL14:0 (myristic acid)</b>	Lipid	Mole % Total Fatty Acid	0.14	0.17	0.76
<b>2-hydroxybutyrate (AHB)</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.14	0.17	0.76
<b>gamma-glutamylisoleucine*</b>	Peptide	Gamma-glutamyl Amino Acid	0.09	0.17	0.76
<b>homocitrulline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.18	0.17	0.76
<b>gamma-glutamyl-2-aminobutyrate</b>	Peptide	Gamma-glutamyl Amino Acid	0.25	0.18	0.76
<b>1,6-anhydroglucose</b>	Xenobiotics	Food Component/Plant	-0.30	0.18	0.76
<b>gamma-glutamylvaline</b>	Peptide	Gamma-glutamyl Amino Acid	0.07	0.18	0.76
<b>inosine</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.41	0.18	0.76
<b>2-aminoheptanoate</b>	Lipid	Fatty Acid, Amino	0.13	0.18	0.76
<b>creatine</b>	Amino Acid	Creatine Metabolism	0.15	0.18	0.76
<b>3-(4-hydroxyphenyl)propionate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.51	0.18	0.76
<b>docosapentaenoate (DPA; 22:5n3)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.14	0.18	0.76

<b>5-oxoproline</b>	Amino Acid	Glutathione Metabolism	-0.11	0.18	0.76
<b>1-myristoylglycerol (14:0)</b>	Lipid	Monoacylglycerol	0.20	0.18	0.76
<b>2-methylmalonyl carnitine</b>	Lipid	Fatty Acid Synthesis	-0.11	0.19	0.76
<b>oxalate (ethanedioate)</b>	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	-0.21	0.19	0.76
<b>2-keto-3-deoxy-gluconate</b>	Xenobiotics	Food Component/Plant	0.17	0.19	0.76
<b>1,5-anhydroglucitol (1,5-AG)</b>	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	-0.19	0.19	0.76
<b>hydantoin-5-propionic acid</b>	Amino Acid	Histidine Metabolism	0.30	0.19	0.76
<b>homostachydrine*</b>	Xenobiotics	Food Component/Plant	-0.17	0.19	0.76
<b>butyrylcarnitine (C4)</b>	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.15	0.19	0.76
<b>N-methylproline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.33	0.20	0.77
<b>orotidine</b>	Nucleotide	Pyrimidine Metabolism, Orotate containing	0.29	0.20	0.77
<b>aspartylphenylalanine</b>	Peptide	Dipeptide	0.29	0.20	0.77
<b>sorbitol</b>	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.21	0.20	0.77
<b>taurocholenate sulfate</b>	Lipid	Secondary Bile Acid Metabolism	-0.22	0.20	0.77
<b>thyroxine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.35	0.20	0.77
<b>arabinose</b>	Carbohydrate	Pentose Metabolism	0.28	0.20	0.77
<b>N-acetylmethionine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.20	0.20	0.77
<b>methyl indole-3-acetate</b>	Xenobiotics	Food Component/Plant	0.19	0.21	0.77
<b>methylsuccinate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.09	0.21	0.77
<b>oleamide</b>	Lipid	Fatty Acid, Amide	0.23	0.21	0.77
<b>gamma-CEHC glucuronide*</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.39	0.21	0.77
<b>2'-deoxyuridine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.17	0.21	0.77
<b>prolylhydroxyproline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.16	0.21	0.77
<b>pyridoxine (Vitamin B6)</b>	Cofactors and Vitamins	Vitamin B6 Metabolism	-0.11	0.21	0.77
<b>5-HETE</b>	Lipid	Eicosanoid	0.22	0.21	0.78
<b>5-methylthioadenosine (MTA)</b>	Amino Acid	Polyamine Metabolism	0.38	0.22	0.78
<b>7-dehydro-cholesterol</b>	Lipid	Sterol	0.44	0.22	0.78
<b>4-methyl-2-oxopentanoate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.08	0.22	0.78
<b>stearoyl-arachidonoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	-0.24	0.22	0.78
<b>oleoylcarnitine (C18)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.15	0.22	0.78
<b>1-linoleoylglycerol (18:2)</b>	Lipid	Monoacylglycerol	0.13	0.22	0.78
<b>gluconate</b>	Xenobiotics	Food Component/Plant	0.10	0.22	0.78
<b>pyroglutamine*</b>	Amino Acid	Glutamate Metabolism	-0.18	0.23	0.78

<b>N-oleoyltaurine</b>	Lipid	Endocannabinoid	0.29	0.23	0.79
<b>1-palmitoylglycerol (16:0)</b>	Lipid	Monoacylglycerol	0.11	0.23	0.79
<b>tyrosylglutamate</b>	Peptide	Dipeptide	0.32	0.23	0.79
<b>beta-tocopherol</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.26	0.23	0.79
<b>alanine</b>	Amino Acid	Alanine and Aspartate Metabolism	0.06	0.23	0.79
<b>inositol 1-phosphate (I1P)</b>	Lipid	Inositol Metabolism	0.13	0.24	0.79
<b>TLTL (Total Total Lipid)</b>	Lipid	Quantitative Total Fatty Acid	0.10	0.24	0.79
<b>N6-methyladenosine</b>	Nucleotide	Purine Metabolism, Adenine containing	0.12	0.24	0.79
<b>N-acetyl-aspartyl-glutamate (NAAG)</b>	Amino Acid	Glutamate Metabolism	-0.09	0.24	0.80
<b>3-methoxycatechol sulfate (1)</b>	Xenobiotics	Benzoate Metabolism	-0.43	0.24	0.80
<b>leucylalanine</b>	Peptide	Dipeptide	0.28	0.25	0.81
<b>glutaryl carnitine (C5)</b>	Amino Acid	Lysine Metabolism	0.08	0.25	0.81
<b>indolebutyrate</b>	Amino Acid	Tryptophan Metabolism	0.24	0.25	0.81
<b>caprylate (8:0)</b>	Lipid	Medium Chain Fatty Acid	-0.07	0.25	0.81
<b>desmosterol</b>	Lipid	Sterol	-0.20	0.25	0.81
<b>4-hydroxyphenylpyruvate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.15	0.25	0.81
<b>erythronate*</b>	Carbohydrate	Aminosugar Metabolism	0.07	0.25	0.81
<b>allo-isoleucine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.08	0.26	0.81
<b>gamma-glutamylleucine</b>	Peptide	Gamma-glutamyl Amino Acid	0.06	0.26	0.81
<b>tartronate (hydroxymalonate)</b>	Xenobiotics	Bacterial/Fungal	-0.17	0.26	0.81
<b>catechol sulfate</b>	Xenobiotics	Benzoate Metabolism	-0.24	0.26	0.81
<b>1,2-propanediol</b>	Xenobiotics	Chemical	0.25	0.26	0.81
<b>threonate</b>	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	-0.18	0.26	0.81
<b>gamma-glutamyllysine</b>	Peptide	Gamma-glutamyl Amino Acid	0.09	0.26	0.81
<b>arabonate</b>	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.11	0.26	0.81
<b>N-delta-acetylornithine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.16	0.27	0.81
<b>3-methoxytyramine sulfate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.13	0.27	0.81
<b>histidyltryptophan</b>	Peptide	Dipeptide	-0.23	0.27	0.81
<b>TL14:1n5 (mystoleic acid)</b>	Lipid	Mole % Total Fatty Acid	0.18	0.27	0.82
<b>gamma-tocopherol</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.16	0.27	0.82
<b>12-HETE</b>	Lipid	Eicosanoid	-0.28	0.28	0.82
<b>docosadienoate (22:2n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.09	0.28	0.82
<b>cyclo(pro-pro)</b>	Peptide	Dipeptide	0.13	0.28	0.82
<b>4-acetamidobutanoate</b>	Amino Acid	Polyamine Metabolism	0.08	0.28	0.82

<b>1-dihomo-linolenylglycerol (alpha, gamma)</b>	Lipid	Monoacylglycerol	0.11	0.28	0.82
<b>glycolithocholate sulfate*</b>	Lipid	Secondary Bile Acid Metabolism	-0.29	0.28	0.82
<b>dopamine sulfate (1)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.18	0.28	0.82
<b>5alpha-pregnan-3beta,20beta-diol monosulfate (1)</b>	Lipid	Steroid	-0.25	0.29	0.82
<b>glycylvaline</b>	Peptide	Dipeptide	0.41	0.29	0.82
<b>isobutyrylglycine (C4)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.12	0.29	0.82
<b>10-nonadecenoate (19:1n9)</b>	Lipid	Long Chain Fatty Acid	0.10	0.29	0.82
<b>TL22:6n3 (docosahexaenoic acid)</b>	Lipid	Mole % Total Fatty Acid	0.10	0.29	0.82
<b>2-arachidonoylglycerophosphoinositol*</b>	Lipid	Lysolipid	0.23	0.29	0.82
<b>alpha-tocopherol</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.11	0.29	0.82
<b>threonylphenylalanine</b>	Peptide	Dipeptide	-0.42	0.29	0.82
<b>3-hydroxydecanoate</b>	Lipid	Fatty Acid, Monohydroxy	-0.10	0.29	0.82
<b>glycerophosphoethanolamine</b>	Lipid	Phospholipid Metabolism	0.16	0.30	0.82
<b>isovalerate (C5)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.09	0.30	0.82
<b>TL24:1n9 (nervonic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.10	0.30	0.82
<b>phenylalanylserine</b>	Peptide	Dipeptide	-0.35	0.30	0.82
<b>octadecanedioate (C18)</b>	Lipid	Fatty Acid, Dicarboxylate	-0.13	0.30	0.82
<b>10-undecenoate (11:1n1)</b>	Lipid	Medium Chain Fatty Acid	-0.10	0.30	0.82
<b>maleate (cis-Butenedioate)</b>	Lipid	Fatty Acid, Dicarboxylate	0.15	0.31	0.82
<b>4-methylcatechol sulfate</b>	Xenobiotics	Benzoate Metabolism	-0.25	0.31	0.82
<b>N-acetylcarnosine</b>	Peptide	Dipeptide Derivative	-0.08	0.31	0.82
<b>2-hydroxypalmitate</b>	Lipid	Fatty Acid, Monohydroxy	-0.06	0.31	0.83
<b>adenosine</b>	Nucleotide	Purine Metabolism, Adenine containing	-0.18	0.31	0.83
<b>paraxanthine</b>	Xenobiotics	Xanthine Metabolism	-0.49	0.32	0.83
<b>1-linoleoyl-GPE (18:2)*</b>	Lipid	Lysolipid	0.09	0.32	0.83
<b>biliverdin</b>	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-0.20	0.32	0.83
<b>bilirubin (E,E)*</b>	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	0.17	0.32	0.83
<b>tryptophylglutamate</b>	Peptide	Dipeptide	-0.39	0.32	0.83
<b>3-hydroxybutyrate (BHBA)</b>	Lipid	Ketone Bodies	-0.20	0.32	0.83
<b>delta-tocopherol</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.23	0.32	0.84
<b>hydroquinone sulfate</b>	Xenobiotics	Drug	-0.28	0.32	0.84
<b>oleoyl-linoleoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	0.05	0.33	0.84
<b>seryltyrosine</b>	Peptide	Dipeptide	0.23	0.33	0.84
<b>nonadecanoate (19:0)</b>	Lipid	Long Chain Fatty Acid	0.06	0.33	0.84

<b>methionine sulfoxide</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.08	0.33	0.84
<b>17-methylstearate</b>	Lipid	Fatty Acid, Branched	0.10	0.33	0.84
<b>palmitate (16:0)</b>	Lipid	Long Chain Fatty Acid	0.05	0.34	0.85
<b>o-cresol sulfate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.54	0.34	0.85
<b>docosapentaenoate (n6 DPA; 22:5n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.07	0.34	0.85
<b>mannitol</b>	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.29	0.35	0.86
<b>N-acetylisoleucine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.14	0.35	0.86
<b>N-acetylneuraminate</b>	Carbohydrate	Aminosugar Metabolism	0.10	0.35	0.86
<b>1-arachidonoylglycerophosphate</b>	Lipid	Lysolipid	0.11	0.35	0.86
<b>TL20:4n6 (arachidonic acid)</b>	Lipid	Mole % Total Fatty Acid	0.06	0.35	0.86
<b>3-(3-hydroxyphenyl)propionate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.37	0.36	0.87
<b>dimethyl sulfone</b>	Xenobiotics	Chemical	0.30	0.36	0.87
<b>12,13-DiHOME</b>	Lipid	Fatty Acid, Dihydroxy	-0.13	0.36	0.88
<b>lysine</b>	Amino Acid	Lysine Metabolism	0.04	0.36	0.88
<b>hypotaurine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.19	0.36	0.88
<b>3-hydroxyisobutyrate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.08	0.37	0.88
<b>16a-hydroxy DHEA 3-sulfate</b>	Lipid	Steroid	-0.17	0.37	0.88
<b>3-methyl-2-oxovalerate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.05	0.37	0.88
<b>cyclohexanebutanoic acid</b>	Xenobiotics	Chemical	-0.10	0.37	0.88
<b>glucuronate</b>	Carbohydrate	Aminosugar Metabolism	0.09	0.37	0.88
<b>methyl-4-hydroxybenzoate sulfate</b>	Xenobiotics	Benzoate Metabolism	-0.37	0.37	0.88
<b>16-hydroxypalmitate</b>	Lipid	Fatty Acid, Monohydroxy	-0.06	0.37	0.88
<b>5alpha-androstan-3beta,17beta-diol disulfate</b>	Lipid	Steroid	-0.23	0.37	0.88
<b>1-methylhistidine</b>	Amino Acid	Histidine Metabolism	0.09	0.38	0.88
<b>indolelactate</b>	Amino Acid	Tryptophan Metabolism	0.06	0.38	0.88
<b>betonicine</b>	Xenobiotics	Food Component/Plant	-0.45	0.38	0.88
<b>glycocholate</b>	Lipid	Primary Bile Acid Metabolism	0.24	0.38	0.88
<b>7-HOCA</b>	Lipid	Sterol	0.09	0.39	0.89
<b>gamma-glutamylphenylalanine</b>	Peptide	Gamma-glutamyl Amino Acid	0.05	0.39	0.89
<b>lactate</b>	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.05	0.39	0.89
<b>arachidate (20:0)</b>	Lipid	Long Chain Fatty Acid	0.05	0.39	0.89
<b>TL22:1n9 (erucic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.18	0.39	0.89
<b>eicosenoyl sphingomyelin*</b>	Lipid	Sphingolipid Metabolism	0.07	0.39	0.89
<b>succinate</b>	Energy	TCA Cycle	-0.04	0.40	0.89

<b>N-acetyl-3-methylhistidine*</b>	Amino Acid	Histidine Metabolism	0.24	0.40	0.89
<b>serine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.05	0.40	0.89
<b>cyclo(gly-pro)</b>	Peptide	Dipeptide	0.13	0.40	0.89
<b>2-piperidinone</b>	Xenobiotics	Food Component/Plant	0.23	0.41	0.89
<b>1,3,7-trimethylurate</b>	Xenobiotics	Xanthine Metabolism	-0.28	0.41	0.89
<b>prolylglycine</b>	Peptide	Dipeptide	-0.15	0.41	0.89
<b>TL18:1n9 (oleic acid)</b>	Lipid	Mole % Total Fatty Acid	0.03	0.41	0.89
<b>methylpalmitate (15 or 2)</b>	Lipid	Fatty Acid, Branched	0.07	0.41	0.89
<b>linoleoylcarnitine*</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.11	0.41	0.89
<b>glycylphenylalanine</b>	Peptide	Dipeptide	-0.22	0.41	0.89
<b>valylarginine</b>	Peptide	Dipeptide	0.21	0.41	0.89
<b>TL18:3n3 (a-linolenic acid)</b>	Lipid	Mole % Total Fatty Acid	0.06	0.41	0.89
<b>pregnenolone sulfate</b>	Lipid	Steroid	0.17	0.42	0.89
<b>palmitoyl-linoleoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	-0.06	0.42	0.89
<b>theobromine</b>	Xenobiotics	Xanthine Metabolism	-0.25	0.42	0.89
<b>saccharin</b>	Xenobiotics	Food Component/Plant	0.48	0.42	0.89
<b>3beta,7alpha-dihydroxy-5-cholestenoate</b>	Lipid	Secondary Bile Acid Metabolism	0.25	0.42	0.89
<b>N-formylmethionine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.04	0.43	0.89
<b>homovanillate (HVA)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.09	0.43	0.89
<b>I-urobilinogen</b>	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	0.35	0.43	0.89
<b>ribose</b>	Carbohydrate	Pentose Metabolism	-0.13	0.43	0.89
<b>gamma-CEHC</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.11	0.43	0.89
<b>dihomolinoleate (20:2n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.07	0.43	0.89
<b>N-acetylglutamine</b>	Amino Acid	Glutamate Metabolism	-0.09	0.43	0.89
<b>3-hydroxyhippurate</b>	Xenobiotics	Benzoate Metabolism	-0.27	0.43	0.89
<b>7-methylurate</b>	Xenobiotics	Xanthine Metabolism	-0.36	0.44	0.89
<b>palmitoyl-linoleoyl-glycerophosphocholine (2)*</b>	Lipid	Lysolipid	-0.05	0.44	0.89
<b>glycerol 3-phosphate (G3P)</b>	Lipid	Glycerolipid Metabolism	0.18	0.44	0.89
<b>N-acetylaspartate (NAA)</b>	Amino Acid	Alanine and Aspartate Metabolism	-0.05	0.44	0.89
<b>kynurenate</b>	Amino Acid	Tryptophan Metabolism	-0.08	0.44	0.89
<b>octanoylcarnitine (C8)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.07	0.44	0.89
<b>asparagine</b>	Amino Acid	Alanine and Aspartate Metabolism	-0.03	0.44	0.89
<b>cis-Cyclo[L-ala-L-Pro]</b>	Peptide	Dipeptide	0.07	0.44	0.89

<b>3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)</b>	Lipid	Fatty Acid, Dicarboxylate	0.28	0.45	0.89
<b>tauroolithocholate 3-sulfate</b>	Lipid	Secondary Bile Acid Metabolism	-0.26	0.45	0.89
<b>trigonelline (N'-methylnicotinate)</b>	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-0.18	0.45	0.89
<b>pantothenate (Vitamin B5)</b>	Cofactors and Vitamins	Pantothenate and CoA Metabolism	0.09	0.45	0.89
<b>acisoga</b>	Amino Acid	Polyamine Metabolism	0.07	0.45	0.89
<b>glycine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.06	0.45	0.89
<b>malate</b>	Energy	TCA Cycle	-0.06	0.45	0.89
<b>1-palmitoleoyl-GPI* (16:1)*</b>	Lipid	Lysolipid	0.33	0.45	0.89
<b>pseudouridine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.04	0.46	0.90
<b>erythritol</b>	Xenobiotics	Food Component/Plant	0.09	0.47	0.90
<b>4-androsten-3beta,17beta-diol monosulfate (1)</b>	Lipid	Steroid	0.15	0.47	0.90
<b>cis-4-decenoyl carnitine</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.07	0.47	0.90
<b>TL18:0 (stearic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.03	0.47	0.90
<b>urea</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.06	0.47	0.90
<b>eicosenoate (20:1n9 or 1n11)</b>	Lipid	Long Chain Fatty Acid	0.07	0.47	0.90
<b>gamma-glutamylmethionine</b>	Peptide	Gamma-glutamyl Amino Acid	0.07	0.47	0.90
<b>androsterone sulfate</b>	Lipid	Steroid	-0.18	0.47	0.90
<b>1-palmitoylglycerophosphate</b>	Lipid	Lysolipid	0.11	0.48	0.90
<b>TL22:4n6 (adrenic acid)</b>	Lipid	Mole % Total Fatty Acid	0.06	0.48	0.90
<b>1,3-dimethylurate</b>	Xenobiotics	Xanthine Metabolism	-0.30	0.48	0.90
<b>dihydroorotate</b>	Nucleotide	Pyrimidine Metabolism, Orotate containing	0.17	0.48	0.90
<b>palmitoyl-linoleoyl-glycerophosphoinositol (1)*</b>	Lipid	Lysolipid	0.14	0.48	0.90
<b>cyclo(L-phe-L-pro)</b>	Peptide	Dipeptide	-0.15	0.48	0.90
<b>maltose</b>	Carbohydrate	Glycogen Metabolism	0.18	0.48	0.90
<b>caffeine</b>	Xenobiotics	Xanthine Metabolism	-0.32	0.48	0.90
<b>ornithine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.06	0.49	0.90
<b>TL22:5n6 (osbond acid)</b>	Lipid	Mole % Total Fatty Acid	0.07	0.49	0.90
<b>salicyluric glucuronide*</b>	Xenobiotics	Drug	0.37	0.49	0.90
<b>margarate (17:0)</b>	Lipid	Long Chain Fatty Acid	0.06	0.49	0.90
<b>2-hydroxyoctanoate</b>	Lipid	Fatty Acid, Monohydroxy	0.08	0.49	0.90
<b>alpha-glutamyltyrosine</b>	Peptide	Dipeptide	-0.23	0.49	0.90
<b>lanosterol</b>	Lipid	Sterol	-0.18	0.49	0.90
<b>5alpha-pregnan-3beta,20alpha-diol disulfate</b>	Lipid	Steroid	0.14	0.49	0.90
<b>1-linoleoyl-GPI* (18:2)*</b>	Lipid	Lysolipid	0.07	0.49	0.90

<b>leucylglycine</b>	Peptide	Dipeptide	-0.24	0.49	0.90
<b>3-(4-hydroxyphenyl)lactate (HPLA)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.04	0.50	0.90
<b>isoleucylglycine</b>	Peptide	Dipeptide	-0.15	0.50	0.90
<b>10-heptadecenoate (17:1n7)</b>	Lipid	Long Chain Fatty Acid	0.07	0.50	0.90
<b>serylalanine</b>	Peptide	Dipeptide	0.11	0.50	0.90
<b>xanthine</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.07	0.50	0.90
<b>arabitol</b>	Carbohydrate	Pentose Metabolism	0.05	0.50	0.90
<b>5alpha-androstan-3beta,17alpha-diol disulfate</b>	Lipid	Steroid	-0.20	0.50	0.90
<b>2-linolenoylglycerophosphocholine (18:3n3)*</b>	Lipid	Lysolipid	-0.21	0.51	0.90
<b>palmitoyl-oleoyl-glycerophosphoglycerol (2)*</b>	Lipid	Lysolipid	0.22	0.51	0.90
<b>3beta,7beta-dihydroxy-5-cholestenoate</b>	Lipid	Sterol	-0.06	0.51	0.90
<b>TL20:2n6 (eicosadienoic acid)</b>	Lipid	Mole % Total Fatty Acid	0.05	0.51	0.90
<b>1-oleoyl-GPI (18:1)*</b>	Lipid	Lysolipid	0.08	0.51	0.90
<b>3-methylhistidine</b>	Amino Acid	Histidine Metabolism	0.16	0.51	0.91
<b>threitol</b>	Carbohydrate	Pentose Metabolism	-0.08	0.52	0.91
<b>1-arachidonoyl-GPI* (20:4)*</b>	Lipid	Lysolipid	0.05	0.52	0.91
<b>taurine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.06	0.52	0.91
<b>theophylline</b>	Xenobiotics	Xanthine Metabolism	-0.26	0.52	0.91
<b>methionine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.03	0.52	0.91
<b>N-palmitoyl glycine</b>	Lipid	Fatty Acid Metabolism(Acyl Glycine)	-0.08	0.52	0.91
<b>5-methyluridine (ribothymidine)</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.04	0.52	0.91
<b>gamma-glutamylglutamate</b>	Peptide	Gamma-glutamyl Amino Acid	0.10	0.53	0.91
<b>O-methylcatechol sulfate</b>	Xenobiotics	Benzoate Metabolism	-0.13	0.53	0.91
<b>2-hydroxystearate</b>	Lipid	Fatty Acid, Monohydroxy	-0.03	0.54	0.91
<b>palmitoyl-palmitoyl-glycerophosphocholine (2)*</b>	Lipid	Lysolipid	0.07	0.54	0.91
<b>ergothioneine</b>	Xenobiotics	Food Component/Plant	0.12	0.54	0.91
<b>3-indoxyl sulfate</b>	Amino Acid	Tryptophan Metabolism	0.10	0.54	0.91
<b>uridine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.03	0.54	0.91
<b>linolenate (18:3n3 or 3n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.06	0.54	0.91
<b>TL20:0 (arachidic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.04	0.54	0.91
<b>pyroglutamylglutamine</b>	Peptide	Dipeptide	0.10	0.54	0.91
<b>4-androsten-3beta,17beta-diol disulfate (2)</b>	Lipid	Steroid	-0.09	0.54	0.91



<b>1,7-dimethylurate</b>	Xenobiotics	Xanthine Metabolism	-0.24	0.54	0.91
<b>vanillylmandelate (VMA)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.07	0.55	0.92
<b>beta-alanine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.06	0.55	0.92
<b>hydroxybutyrylcarnitine*</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.11	0.55	0.92
<b>myristate (14:0)</b>	Lipid	Long Chain Fatty Acid	0.05	0.56	0.92
<b>stearoyl-arachidonoyl-glycerophosphoinositol (1)*</b>	Lipid	Lysolipid	0.04	0.56	0.93
<b>fructose</b>	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.05	0.57	0.93
<b>N-acetylserine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	0.03	0.57	0.93
<b>1-methylimidazoleacetate</b>	Amino Acid	Histidine Metabolism	0.10	0.57	0.93
<b>2-aminoadipate</b>	Amino Acid	Lysine Metabolism	0.05	0.57	0.93
<b>imidazole lactate</b>	Amino Acid	Histidine Metabolism	0.05	0.57	0.93
<b>phenylacetate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.09	0.57	0.93
<b>glycylproline</b>	Peptide	Dipeptide	0.14	0.57	0.93
<b>phenylcarnitine*</b>	Xenobiotics	Chemical	-0.18	0.57	0.93
<b>pyroglutamylvaline</b>	Peptide	Dipeptide	-0.05	0.58	0.93
<b>oleic ethanolamide</b>	Lipid	Endocannabinoid	-0.05	0.58	0.93
<b>tryptophan betaine</b>	Amino Acid	Tryptophan Metabolism	-0.15	0.58	0.93
<b>glycylglycine</b>	Peptide	Dipeptide	-0.24	0.58	0.93
<b>N-methylpipercolate</b>	Xenobiotics	Chemical	-0.10	0.58	0.93
<b>2-oleoylglycerol (18:1)</b>	Lipid	Monoacylglycerol	0.06	0.58	0.93
<b>4-hydroxychlorothalonil</b>	Xenobiotics	Chemical	0.08	0.58	0.93
<b>2-aminobutyrate</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.05	0.59	0.93
<b>HWESASXX*</b>	Peptide	Polypeptide	-0.12	0.59	0.93
<b>TL20:3n6 (di-homo-g-linoleic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.03	0.59	0.93
<b>glycochenodeoxycholate</b>	Lipid	Primary Bile Acid Metabolism	0.13	0.59	0.93
<b>fumarate</b>	Energy	TCA Cycle	-0.05	0.59	0.93
<b>cyclo(leu-pro)</b>	Peptide	Dipeptide	-0.10	0.59	0.93
<b>cholestanol</b>	Lipid	Sterol	-0.05	0.60	0.94
<b>5alpha-androstan-3alpha,17beta-diol disulfate</b>	Lipid	Steroid	-0.18	0.60	0.94
<b>choline</b>	Lipid	Phospholipid Metabolism	0.03	0.60	0.94
<b>phenylacetylglutamine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.09	0.60	0.94
<b>4-androsten-3beta,17beta-diol monosulfate (2)</b>	Lipid	Steroid	-0.13	0.60	0.94
<b>1-oleoylglycerol (18:1)</b>	Lipid	Monoacylglycerol	0.06	0.61	0.94
<b>4-guanidinobutanoate</b>	Amino Acid	Guanidino and Acetamido Metabolism	-0.16	0.61	0.94

<b>5alpha-pregnan-3beta,20alpha-diol monosulfate (2)</b>	Lipid	Steroid	0.19	0.61	0.94
<b>erucate (22:1n9)</b>	Lipid	Long Chain Fatty Acid	0.05	0.61	0.94
<b>N-acetyltaurine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.06	0.61	0.94
<b>sphingomyelin</b>	Lipid	Sphingolipid Metabolism	0.04	0.61	0.94
<b>3-methoxycatechol sulfate (2)</b>	Xenobiotics	Benzoate Metabolism	-0.14	0.62	0.94
<b>2,3-dihydroxyisovalerate</b>	Xenobiotics	Food Component/Plant	0.17	0.62	0.94
<b>glycocholenate sulfate*</b>	Lipid	Secondary Bile Acid Metabolism	-0.05	0.62	0.94
<b>3-[3-(sulfooxy)phenyl]propanoic acid</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.23	0.62	0.94
<b>5,6-dihydrouracil</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.04	0.62	0.94
<b>allantoin</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.08	0.62	0.94
<b>oleoyl sphingomyelin</b>	Lipid	Sphingolipid Metabolism	0.03	0.62	0.94
<b>cysteine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.05	0.62	0.94
<b>tyrosine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.03	0.62	0.94
<b>2-pyrrolidinone</b>	Xenobiotics	Chemical	0.09	0.63	0.94
<b>isobutyrylcarnitine (C4)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.06	0.63	0.94
<b>4-androsten-3beta,17beta-diol disulfate (1)</b>	Lipid	Steroid	0.10	0.63	0.94
<b>pyridoxal</b>	Cofactors and Vitamins	Vitamin B6 Metabolism	-0.17	0.63	0.94
<b>TLdm18:1n7 (plasmalogen vaccenic acid)</b>	Lipid	Mole % Total Fatty Acid	0.10	0.64	0.94
<b>N2,N5-diacetylornithine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.10	0.64	0.94
<b>1-methylguanosine</b>	Nucleotide	Purine Metabolism, Guanine containing	-0.02	0.64	0.94
<b>threonine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.03	0.64	0.94
<b>isovalerylglycine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.06	0.65	0.95
<b>N-acetylalanine</b>	Amino Acid	Alanine and Aspartate Metabolism	0.02	0.65	0.95
<b>aspartylleucine</b>	Peptide	Dipeptide	-0.07	0.65	0.95
<b>aspartate</b>	Amino Acid	Alanine and Aspartate Metabolism	0.05	0.65	0.95
<b>decanoylcarnitine (C10)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.04	0.65	0.95
<b>gamma-glutamylglutamine</b>	Peptide	Gamma-glutamyl Amino Acid	-0.04	0.65	0.95
<b>valerylcarnitine (C5)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.17	0.66	0.95
<b>ADSGEGDFXAEGGGVR*</b>	Peptide	Fibrinogen Cleavage Peptide	0.04	0.66	0.95
<b>cinnamoylglycine</b>	Xenobiotics	Food Component/Plant	0.22	0.66	0.95
<b>myristoleoyl sphingomyelin*</b>	Lipid	Sphingolipid Metabolism	-0.05	0.66	0.95

<b>1-methylurate</b>	Xenobiotics	Xanthine Metabolism	-0.11	0.67	0.95
<b>andro steroid monosulfate (1)*</b>	Lipid	Steroid	-0.12	0.67	0.95
<b>phenol sulfate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.12	0.67	0.95
<b>palmitoleate (16:1n7)</b>	Lipid	Long Chain Fatty Acid	0.05	0.67	0.95
<b>N-acetylhistidine</b>	Amino Acid	Histidine Metabolism	-0.09	0.67	0.95
<b>N-acetylcitrulline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.11	0.67	0.95
<b>pregnen-diol disulfate*</b>	Lipid	Steroid	0.07	0.67	0.95
<b>3-hydroxylaurate</b>	Lipid	Fatty Acid, Monohydroxy	-0.04	0.67	0.95
<b>indoleacetate</b>	Amino Acid	Tryptophan Metabolism	0.05	0.68	0.95
<b>5alpha-pregnan-3(alpha or beta),20beta-diol disulfate</b>	Lipid	Steroid	-0.21	0.68	0.95
<b>pelargonate (9:0)</b>	Lipid	Medium Chain Fatty Acid	-0.02	0.68	0.95
<b>deoxycarnitine</b>	Lipid	Carnitine Metabolism	-0.02	0.68	0.95
<b>glucarate 1,4-lactone</b>	Carbohydrate	Disaccharides and Oligosaccharides	-0.29	0.68	0.95
<b>guanosine</b>	Nucleotide	Purine Metabolism, Guanine containing	-0.14	0.68	0.95
<b>proline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.02	0.68	0.95
<b>1-palmitoyl-GPI* (16:0)*</b>	Lipid	Lysolipid	0.06	0.68	0.95
<b>glycerophosphorylcholine (GPC)</b>	Lipid	Phospholipid Metabolism	0.03	0.69	0.95
<b>taurocholate</b>	Lipid	Primary Bile Acid Metabolism	0.15	0.69	0.95
<b>2-hydroxyhippurate (salicylurate)</b>	Xenobiotics	Benzoate Metabolism	0.16	0.69	0.95
<b>TL22:0 (behenic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.04	0.69	0.96
<b>hydroxyproline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.05	0.70	0.96
<b>3-hydroxypyridine sulfate</b>	Xenobiotics	Chemical	0.11	0.70	0.96
<b>4-ethylphenyl sulfate</b>	Xenobiotics	Benzoate Metabolism	0.09	0.70	0.96
<b>myristoleoylcarnitine*</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.06	0.70	0.96
<b>isovalerylcarnitine (C5)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.04	0.71	0.96
<b>citrulline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.03	0.71	0.96
<b>glycerol</b>	Lipid	Glycerolipid Metabolism	0.03	0.71	0.96
<b>lathosterol</b>	Lipid	Sterol	0.06	0.71	0.96
<b>beta-hydroxyisovaleroylcarnitine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.03	0.71	0.96
<b>TL24:0 (lignoceric acid)</b>	Lipid	Mole % Total Fatty Acid	0.05	0.71	0.96
<b>campesterol</b>	Lipid	Sterol	0.05	0.72	0.96
<b>ursodeoxycholate</b>	Lipid	Secondary Bile Acid Metabolism	0.14	0.72	0.96
<b>gamma-glutamyltryptophan</b>	Peptide	Gamma-glutamyl Amino Acid	0.03	0.72	0.96
<b>TLdm18:1n9 (plasmalogen oleic acid)</b>	Lipid	Mole % Total Fatty Acid	0.04	0.72	0.96

<b>2-hydroxydecanoate</b>	Lipid	Fatty Acid, Monohydroxy	0.04	0.72	0.96
<b>N2-acetyllysine</b>	Amino Acid	Lysine Metabolism	-0.06	0.72	0.96
<b>acetoacetate</b>	Lipid	Ketone Bodies	-0.05	0.73	0.96
<b>kynurenine</b>	Amino Acid	Tryptophan Metabolism	0.02	0.73	0.96
<b>myo-inositol</b>	Lipid	Inositol Metabolism	0.02	0.73	0.96
<b>guanidinoacetate</b>	Amino Acid	Creatine Metabolism	0.03	0.73	0.96
<b>linoleate (18:2n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.02	0.73	0.96
<b>glycolate (hydroxyacetate)</b>	Xenobiotics	Chemical	-0.02	0.73	0.96
<b>dihomolinolenate (20:3n3 or 3n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.02	0.73	0.96
<b>pipecolate</b>	Amino Acid	Lysine Metabolism	-0.05	0.73	0.96
<b>valine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.01	0.74	0.96
<b>ectoine</b>	Xenobiotics	Chemical	0.09	0.74	0.96
<b>hypoxanthine</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.06	0.74	0.96
<b>squalene</b>	Lipid	Sterol	0.10	0.74	0.96
<b>C-glycosyltryptophan</b>	Amino Acid	Tryptophan Metabolism	0.02	0.74	0.96
<b>TL16:0 (palmitic acid)</b>	Lipid	Mole % Total Fatty Acid	0.01	0.74	0.96
<b>quinolinate</b>	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.05	0.74	0.96
<b>3,7-dimethylurate</b>	Xenobiotics	Xanthine Metabolism	-0.11	0.74	0.96
<b>alpha-hydroxyisocaproate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.03	0.74	0.96
<b>coprostanol</b>	Lipid	Sterol	0.10	0.75	0.96
<b>glycoursodeoxycholate</b>	Lipid	Secondary Bile Acid Metabolism	0.11	0.75	0.96
<b>stachydrine</b>	Xenobiotics	Food Component/Plant	-0.10	0.75	0.96
<b>quinat</b>	Xenobiotics	Food Component/Plant	0.16	0.75	0.96
<b>bilirubin</b>	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	0.09	0.75	0.96
<b>acetylcarnitine (C2)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.03	0.75	0.96
<b>cys-gly, oxidized</b>	Amino Acid	Glutathione Metabolism	-0.06	0.75	0.96
<b>TL20:4n3 (eicosatetraenoic acid)</b>	Lipid	Mole % Total Fatty Acid	0.04	0.75	0.96
<b>eicosanodioate</b>	Lipid	Fatty Acid, Dicarboxylate	-0.04	0.76	0.96
<b>indole-3-carboxylic acid</b>	Amino Acid	Tryptophan Metabolism	-0.02	0.76	0.96
<b>adenosine 3',5'-cyclic monophosphate (cAMP)</b>	Nucleotide	Purine Metabolism, Adenine containing	-0.07	0.76	0.96
<b>glutarate (pentanedioate)</b>	Amino Acid	Lysine Metabolism	0.05	0.76	0.96
<b>etiocholanolone glucuronide</b>	Lipid	Steroid	-0.08	0.77	0.96
<b>N2,N2-dimethylguanosine</b>	Nucleotide	Purine Metabolism, Guanine containing	0.02	0.77	0.96
<b>xylose</b>	Carbohydrate	Pentose Metabolism	0.06	0.77	0.96

<b>4-allylphenol sulfate</b>	Xenobiotics	Food Component/Plant	0.07	0.77	0.96
<b>palmitoyl-oleoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	0.02	0.77	0.96
<b>taurodeoxycholate</b>	Lipid	Secondary Bile Acid Metabolism	0.13	0.77	0.96
<b>docosatienoate (22:3n3)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.03	0.77	0.96
<b>adenine</b>	Nucleotide	Purine Metabolism, Adenine containing	0.04	0.77	0.96
<b>hexanoylcarnitine (C6)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.02	0.78	0.96
<b>3-hydroxymyristate</b>	Lipid	Fatty Acid, Monohydroxy	-0.03	0.78	0.96
<b>salicylate</b>	Xenobiotics	Drug	0.12	0.78	0.96
<b>3-methylglutarylcarnitine (1)</b>	Amino Acid	Lysine Metabolism	-0.04	0.78	0.96
<b>palmitoyl ethanolamide</b>	Lipid	Endocannabinoid	-0.02	0.78	0.96
<b>1-docosapentaenoyl-GPC* (22:5n6)*</b>	Lipid	Lysolipid	-0.09	0.78	0.96
<b>palmitoleoyl sphingomyelin*</b>	Lipid	Sphingolipid Metabolism	0.01	0.79	0.96
<b>1-pentadecanoylglycerol (1-monopentadecanoin)</b>	Lipid	Monoacylglycerol	-0.03	0.79	0.96
<b>pentadecanoate (15:0)</b>	Lipid	Long Chain Fatty Acid	0.02	0.79	0.97
<b>glycodeoxycholate</b>	Lipid	Secondary Bile Acid Metabolism	0.11	0.79	0.97
<b>gamma-glutamylhistidine</b>	Peptide	Gamma-glutamyl Amino Acid	0.06	0.80	0.97
<b>scyllo-inositol</b>	Lipid	Inositol Metabolism	-0.04	0.80	0.97
<b>2-stearoylglycerophosphoinositol*</b>	Lipid	Lysolipid	-0.04	0.80	0.97
<b>cystine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.01	0.81	0.97
<b>cortisone</b>	Lipid	Steroid	-0.04	0.81	0.97
<b>glycerate</b>	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	-0.02	0.81	0.97
<b>4-ureidobutyrate</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.04	0.81	0.97
<b>histidine</b>	Amino Acid	Histidine Metabolism	-0.02	0.81	0.97
<b>stearoyl-linoleoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	0.02	0.82	0.97
<b>imidazole propionate</b>	Amino Acid	Histidine Metabolism	0.04	0.82	0.97
<b>pregn steroid monosulfate*</b>	Lipid	Steroid	0.03	0.82	0.97
<b>creatinine</b>	Amino Acid	Creatine Metabolism	0.01	0.82	0.97
<b>2-hydroxyglutarate</b>	Lipid	Fatty Acid, Dicarboxylate	-0.02	0.82	0.97
<b>phenylalanyltryptophan</b>	Peptide	Dipeptide	0.04	0.82	0.97
<b>13-HODE + 9-HODE</b>	Lipid	Fatty Acid, Monohydroxy	-0.03	0.83	0.97
<b>N-(2-furoyl)glycine</b>	Xenobiotics	Food Component/Plant	0.04	0.83	0.97
<b>21-hydroxypregnenolone disulfate</b>	Lipid	Steroid	0.04	0.83	0.97
<b>beta-sitosterol</b>	Lipid	Sterol	0.03	0.83	0.97
<b>TLdm16:0 (plasmalogen palmitic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.02	0.83	0.97

<b>caprate (10:0)</b>	Lipid	Medium Chain Fatty Acid	-0.02	0.83	0.97
<b>xylonate</b>	Carbohydrate	Pentose Metabolism	0.04	0.83	0.97
<b>p-cresol sulfate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.06	0.84	0.97
<b>N3-methyluridine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.03	0.84	0.97
<b>arginine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.01	0.84	0.97
<b>TL15:0 (pentadecanoic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.01	0.84	0.97
<b>2-methylbutyrocarnitine (C5)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.02	0.84	0.97
<b>thymol sulfate</b>	Xenobiotics	Food Component/Plant	0.09	0.84	0.97
<b>gamma-glutamyltyrosine</b>	Peptide	Gamma-glutamyl Amino Acid	-0.01	0.84	0.97
<b>dehydroisoandrosterone sulfate (DHEA-S)</b>	Lipid	Steroid	0.04	0.84	0.97
<b>stearoyl-linoleoyl-glycerophosphocholine (2)*</b>	Lipid	Lysolipid	-0.02	0.84	0.97
<b>O-sulfo-L-tyrosine</b>	Xenobiotics	Chemical	0.01	0.84	0.97
<b>3-phenylpropionate (hydrocinnamate)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.06	0.85	0.97
<b>cholate</b>	Lipid	Primary Bile Acid Metabolism	0.07	0.85	0.97
<b>stearoyl-linoleoyl-glycerophosphoethanolamine (1)*</b>	Lipid	Lysolipid	-0.02	0.85	0.97
<b>pregnanediol-3-glucuronide</b>	Lipid	Steroid	-0.06	0.85	0.97
<b>glycolithocholate</b>	Lipid	Secondary Bile Acid Metabolism	-0.08	0.85	0.98
<b>tryptophan</b>	Amino Acid	Tryptophan Metabolism	0.01	0.86	0.98
<b>N-acetylarginine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.02	0.86	0.98
<b>tiglyl carnitine (C5)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.02	0.86	0.98
<b>palmitoyl-palmitoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	-0.02	0.87	0.98
<b>vaccenate (18:1n7)</b>	Lipid	Long Chain Fatty Acid	0.01	0.87	0.98
<b>taurochenodeoxycholate</b>	Lipid	Primary Bile Acid Metabolism	0.05	0.87	0.98
<b>cholesterol</b>	Lipid	Sterol	-0.01	0.87	0.98
<b>serotonin (5HT)</b>	Amino Acid	Tryptophan Metabolism	0.04	0.87	0.98
<b>palmitoyl-arachidonoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	0.02	0.87	0.98
<b>urate</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.01	0.87	0.98
<b>tyramine O-sulfate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.04	0.87	0.98
<b>pyrraline</b>	Xenobiotics	Food Component/Plant	-0.04	0.88	0.98
<b>N-acetyltyrosine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.02	0.88	0.98
<b>pyridoxate</b>	Cofactors and Vitamins	Vitamin B6 Metabolism	-0.03	0.88	0.98

<b>dimethylglycine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	0.01	0.88	0.98
<b>7-methylguanine</b>	Nucleotide	Purine Metabolism, Guanine containing	-0.01	0.88	0.98
<b>phenylalanylglutamate</b>	Peptide	Dipeptide	0.07	0.89	0.98
<b>13-methylmyristic acid</b>	Lipid	Fatty Acid, Branched	0.01	0.89	0.98
<b>N-acetyl-beta-alanine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.01	0.89	0.98
<b>4-hydroxybenzoate</b>	Xenobiotics	Benzoate Metabolism	0.06	0.89	0.98
<b>phenylalanylphenylalanine</b>	Peptide	Dipeptide	0.02	0.89	0.98
<b>levulinate (4-oxovalerate)</b>	Xenobiotics	Food Component/Plant	-0.01	0.89	0.98
<b>N-acetyl-1-methylhistidine*</b>	Amino Acid	Histidine Metabolism	-0.02	0.90	0.98
<b>7-methylxanthine</b>	Xenobiotics	Xanthine Metabolism	-0.04	0.90	0.98
<b>propionylcarnitine (C3)</b>	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.01	0.90	0.98
<b>TL18:1n7 (avaccenic acid)</b>	Lipid	Mole % Total Fatty Acid	0.01	0.90	0.99
<b>S-adenosylhomocysteine (SAH)</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.02	0.90	0.99
<b>5-acetylamino-6-amino-3-methyluracil</b>	Xenobiotics	Xanthine Metabolism	0.05	0.91	0.99
<b>homoarginine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.03	0.91	0.99
<b>chenodeoxycholate</b>	Lipid	Primary Bile Acid Metabolism	0.03	0.91	0.99
<b>5-dodecenoate (12:1n7)</b>	Lipid	Medium Chain Fatty Acid	-0.01	0.91	0.99
<b>2-linoleoylglycerol (2-monolinolein)</b>	Lipid	Monoacylglycerol	0.02	0.92	0.99
<b>laurylcarnitine (C12)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.01	0.92	0.99
<b>gamma-glutamylthreonine*</b>	Peptide	Gamma-glutamyl Amino Acid	0.01	0.92	0.99
<b>myristoleate (14:1n5)</b>	Lipid	Long Chain Fatty Acid	-0.02	0.92	0.99
<b>oleoyl-linoleoyl-glycerophosphocholine (2)*</b>	Lipid	Lysolipid	0.01	0.92	0.99
<b>4-androsten-3alpha,17alpha-diol monosulfate (3)</b>	Lipid	Steroid	-0.02	0.92	0.99
<b>N1-Methyl-2-pyridone-5-carboxamide</b>	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.01	0.92	0.99
<b>gentisate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.04	0.93	0.99
<b>p-cresol-glucuronide*</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.04	0.93	0.99
<b>N-acetylkynurenine (2)</b>	Amino Acid	Tryptophan Metabolism	0.03	0.93	0.99
<b>ribonate (ribonolactone)</b>	Carbohydrate	Pentose Metabolism	0.01	0.93	0.99
<b>oleate (18:1n9)</b>	Lipid	Long Chain Fatty Acid	0.01	0.93	0.99
<b>isoleucine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.004	0.93	0.99
<b>pyroglutamylglycine</b>	Peptide	Dipeptide	0.02	0.94	0.99
<b>N-acetylphenylalanine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.01	0.94	0.99
<b>hippurate</b>	Xenobiotics	Benzoate Metabolism	0.02	0.94	0.99

<b>palmitoyl sphingomyelin</b>	Lipid	Sphingolipid Metabolism	0.003	0.94	0.99
<b>cortisol</b>	Lipid	Steroid	0.01	0.94	0.99
<b>2-aminophenol sulfate</b>	Xenobiotics	Chemical	-0.02	0.94	0.99
<b>nicotinamide</b>	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.01	0.94	0.99
<b>succinylcarnitine (C4)</b>	Energy	TCA Cycle	0.01	0.95	0.99
<b>laurate (12:0)</b>	Lipid	Medium Chain Fatty Acid	0.01	0.95	0.99
<b>tartarate</b>	Xenobiotics	Food Component/Plant	-0.02	0.95	0.99
<b>histidylphenylalanine</b>	Peptide	Dipeptide	0.02	0.95	0.99
<b>N-acetylglutamate</b>	Amino Acid	Glutamate Metabolism	0.01	0.95	0.99
<b>phenylalanine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.002	0.95	0.99
<b>4-androsten-3alpha,17alpha-diol monosulfate (2)</b>	Lipid	Steroid	-0.01	0.96	0.99
<b>3-methylxanthine</b>	Xenobiotics	Xanthine Metabolism	-0.02	0.96	0.99
<b>trans-urocanate</b>	Amino Acid	Histidine Metabolism	0.01	0.96	0.99
<b>5alpha-androstan-3alpha,17beta-diol monosulfate (1)</b>	Lipid	Steroid	0.02	0.96	0.99
<b>DSGEGDFXAEGGGVR*</b>	Peptide	Fibrinogen Cleavage Peptide	-0.01	0.97	1.00
<b>N-6-trimethyllysine</b>	Amino Acid	Lysine Metabolism	-0.004	0.97	1.00
<b>piperine</b>	Xenobiotics	Food Component/Plant	-0.01	0.97	1.00
<b>5-hydroxyindoleacetate</b>	Amino Acid	Tryptophan Metabolism	-0.003	0.97	1.00
<b>deoxycholate</b>	Lipid	Secondary Bile Acid Metabolism	0.01	0.98	1.00
<b>phosphate</b>	Energy	Oxidative Phosphorylation	-0.001	0.98	1.00
<b>TLdm18:0 (plasmalogen stearic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.002	0.98	1.00
<b>1-methylxanthine</b>	Xenobiotics	Xanthine Metabolism	-0.01	0.98	1.00
<b>N6-carbamoylthreonyladenosine</b>	Nucleotide	Purine Metabolism, Adenine containing	0.002	0.98	1.00
<b>leucine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.001	0.98	1.00
<b>1-stearoyl-GPI (18:0)</b>	Lipid	Lysolipid	0.002	0.99	1.00
<b>sphingosine 1-phosphate</b>	Lipid	Sphingolipid Metabolism	0.001	0.99	1.00
<b>carnitine</b>	Lipid	Carnitine Metabolism	-0.001	0.99	1.00
<b>epiandrosterone sulfate</b>	Lipid	Steroid	0.004	0.99	1.00
<b>galactonate</b>	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.01	0.99	1.00
<b>N-acetylalliin</b>	Xenobiotics	Food Component/Plant	-0.01	0.99	1.00
<b>4-vinylphenol sulfate</b>	Xenobiotics	Benzoate Metabolism	-0.003	0.99	1.00
<b>tyrosylglutamine</b>	Peptide	Dipeptide	0.002	0.99	1.00
<b>N-acetylthreonine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	0.001	0.99	1.00
<b>stigmasterol</b>	Lipid	Sterol	-0.001	0.99	1.00



<b>N-acetylvaline</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.0003	1.00	1.00
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\*Covariates: age, sex, diabetes, hypertension, BMI, and liver fibrosis stage  
TCA = tricarboxylic acid cycle; GPE = Glycerophosphoethanolamine; GPC = Glycerophosphocholine; SAM = S-Adenosyl methionine

**Table S4: HFpEF-no fatigue full results\***

Metabolite	Pathway	Sub-Pathway	log Fold change	Unadjusted p-value	Adjusted p-value
1-arachidonoyl-GPE* (20:4)*	Lipid	Lysolipid	0.27	0.0004	0.13
azelate (nonanedioate; C9)	Lipid	Fatty Acid, Dicarboxylate	-0.37	0.0006	0.13
taurocholenate sulfate	Lipid	Secondary Bile Acid Metabolism	-0.60	0.0008	0.13
1-stearoyl-GPE (18:0)	Lipid	Lysolipid	0.28	0.001	0.13
1-arachidonylglycerol	Lipid	Monoacylglycerol	0.30	0.001	0.13
1-docosahexaenoylglycerophosphoethanolamine*	Lipid	Lysolipid	0.35	0.001	0.13
2-stearoylglycerophosphoethanolamine*	Lipid	Lysolipid	0.33	0.001	0.13
1-oleoyl-GPE (18:1)	Lipid	Lysolipid	0.27	0.002	0.15
1-palmitoyl-GPE (16:0)	Lipid	Lysolipid	0.27	0.002	0.18
2-arachidonoyl glycerol	Lipid	Monoacylglycerol	0.32	0.003	0.20
1-linolenylglycerol	Lipid	Monoacylglycerol	0.34	0.004	0.25
citrate	Energy	TCA Cycle	-0.20	0.005	0.26
2-oleoyl-GPE* (18:1)*	Lipid	Lysolipid	0.85	0.007	0.37
7-alpha-hydroxycholesterol	Lipid	Sterol	0.50	0.009	0.37
2-palmitoyl-GPE* (16:0)*	Lipid	Lysolipid	0.31	0.009	0.37
1-eicosatrienoylglycerophosphoethanolamine*	Lipid	Lysolipid	0.65	0.009	0.37
N2-methylguanosine	Nucleotide	Purine Metabolism, Guanine containing	0.28	0.01	0.37
alpha-ketoglutarate	Energy	TCA Cycle	0.29	0.01	0.37
2-arachidonoyl-GPE* (20:4)*	Lipid	Lysolipid	0.50	0.01	0.39
1-docosahexaenoylglycerol	Lipid	Monoacylglycerol	0.36	0.01	0.39
TL18:3n6 (g-linolenic acid)	Lipid	Mole % Total Fatty Acid	0.22	0.01	0.41
2-docosahexaenoylglycerol*	Lipid	Monoacylglycerol	0.85	0.01	0.44
glycerophosphoethanolamine	Lipid	Phospholipid Metabolism	0.38	0.02	0.52
hexanoylglycine (C6)	Lipid	Fatty Acid Metabolism(Acyl Glycine)	0.76	0.02	0.53
N6-acetyllysine	Amino Acid	Lysine Metabolism	0.12	0.02	0.54
methyl glucopyranoside (alpha + beta)	Xenobiotics	Food Component/Plant	-0.72	0.02	0.59
glutamine	Amino Acid	Glutamate Metabolism	-0.09	0.02	0.59
5alpha-pregnan-3beta,20beta-diol monosulfate (1)	Lipid	Steroid	-0.54	0.03	0.59
2-palmitoylglycerol (16:0)	Lipid	Monoacylglycerol	0.36	0.03	0.59
TL14:0 (myristic acid)	Lipid	Mole % Total Fatty Acid	0.23	0.03	0.59

<b>pyruvate</b>	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.33	0.03	0.59
<b>N-delta-acetylornithine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.33	0.03	0.59
<b>1-linoleoylglycerol (18:2)</b>	Lipid	Monoacylglycerol	0.24	0.03	0.59
<b>1-myristoyl-GPC (14:0)</b>	Lipid	Lysolipid	0.32	0.03	0.59
<b>3b-hydroxy-5-choleonoic acid</b>	Lipid	Secondary Bile Acid Metabolism	-0.57	0.03	0.59
<b>arabinose</b>	Carbohydrate	Pentose Metabolism	0.49	0.03	0.59
<b>benzoate</b>	Xenobiotics	Benzoate Metabolism	-0.16	0.04	0.59
<b>1-palmitoylglycerol (16:0)</b>	Lipid	Monoacylglycerol	0.21	0.04	0.59
<b>phenylpyruvate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.17	0.04	0.59
<b>3beta,7alpha-dihydroxy-5-cholestenoate</b>	Lipid	Secondary Bile Acid Metabolism	0.68	0.04	0.59
<b>2-keto-3-deoxy-gluconate</b>	Xenobiotics	Food Component/Plant	0.29	0.04	0.59
<b>1-myristoylglycerol (14:0)</b>	Lipid	Monoacylglycerol	0.32	0.04	0.59
<b>pyridoxine (Vitamin B6)</b>	Cofactors and Vitamins	Vitamin B6 Metabolism	-0.19	0.04	0.59
<b>S-methylcysteine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.21	0.04	0.59
<b>3-methoxytyrosine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.14	0.04	0.60
<b>threonine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.12	0.04	0.60
<b>stearoyl-arachidonoyl-glycerophosphoethanolamine (1)*</b>	Lipid	Lysolipid	0.23	0.04	0.60
<b>1-dihomo-linolenylglycerol (alpha, gamma)</b>	Lipid	Monoacylglycerol	0.22	0.04	0.60
<b>butyrylcarnitine (C4)</b>	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.24	0.05	0.60
<b>orotate</b>	Nucleotide	Pyrimidine Metabolism, Orotate containing	0.34	0.05	0.60
<b>2-oleoylglycerol (18:1)</b>	Lipid	Monoacylglycerol	0.24	0.05	0.64
<b>gamma-CEHC glucuronide*</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.63	0.05	0.64
<b>3-methyl catechol sulfate (1)</b>	Xenobiotics	Benzoate Metabolism	0.63	0.05	0.65
<b>eugenol sulfate</b>	Xenobiotics	Food Component/Plant	0.83	0.05	0.65
<b>methionine sulfone</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.30	0.06	0.65
<b>caproate (6:0)</b>	Lipid	Medium Chain Fatty Acid	-0.12	0.06	0.65
<b>16a-hydroxy DHEA 3-sulfate</b>	Lipid	Steroid	-0.37	0.06	0.65
<b>2-myristoyl-GPC* (14:0)*</b>	Lipid	Lysolipid	0.40	0.06	0.65
<b>4-androsten-3beta,17beta-diol disulfate (2)</b>	Lipid	Steroid	-0.28	0.06	0.65
<b>indoleacetylglutamine</b>	Amino Acid	Tryptophan Metabolism	0.64	0.06	0.65
<b>1-pentadecanoylglycerophosphocholine (15:0)*</b>	Lipid	Lysolipid	0.20	0.06	0.65

<b>alpha-hydroxycaproate</b>	Lipid	Fatty Acid, Monohydroxy	0.16	0.06	0.65
<b>cytidine</b>	Nucleotide	Pyrimidine Metabolism, Cytidine containing	0.18	0.06	0.65
<b>1-oleoylglycerol (18:1)</b>	Lipid	Monoacylglycerol	0.22	0.07	0.66
<b>2-linoleoylglycerol (2-monolinolein)</b>	Lipid	Monoacylglycerol	0.29	0.07	0.66
<b>3-hydroxybutyrate (BHBA)</b>	Lipid	Ketone Bodies	-0.38	0.07	0.66
<b>indolebutyrate</b>	Amino Acid	Tryptophan Metabolism	0.39	0.07	0.66
<b>beta-alanine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.19	0.07	0.66
<b>TL20:3n9 (mead acid)</b>	Lipid	Mole % Total Fatty Acid	0.26	0.07	0.66
<b>5alpha-pregnan-3(alpha or beta),20beta-diol disulfate</b>	Lipid	Steroid	-0.94	0.07	0.66
<b>N-acetylleucine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.16	0.07	0.66
<b>palmitoyl-linoleoyl-glycerophosphocholine (2)*</b>	Lipid	Lysolipid	-0.12	0.08	0.66
<b>gluconate</b>	Xenobiotics	Food Component/Plant	0.15	0.08	0.66
<b>methionine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.09	0.08	0.66
<b>3-(4-hydroxyphenyl)propionate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.70	0.08	0.66
<b>2-docosahexaenoyl-GPC* (22:6)*</b>	Lipid	Lysolipid	0.28	0.08	0.66
<b>gamma-glutamylglutamine</b>	Peptide	Gamma-glutamyl Amino Acid	-0.16	0.08	0.66
<b>biliverdin</b>	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-0.36	0.08	0.66
<b>1-eicosapentaenoylglycerophosphocholine (20:5n3)*</b>	Lipid	Lysolipid	0.33	0.08	0.66
<b>indolepropionate</b>	Amino Acid	Tryptophan Metabolism	-0.35	0.09	0.66
<b>orotidine</b>	Nucleotide	Pyrimidine Metabolism, Orotate containing	0.40	0.09	0.66
<b>propionylglycine (C3)</b>	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.21	0.09	0.66
<b>2-aminobutyrate</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.15	0.09	0.66
<b>methyl indole-3-acetate</b>	Xenobiotics	Food Component/Plant	0.26	0.09	0.66
<b>2-hydroxyglutarate</b>	Lipid	Fatty Acid, Dicarboxylate	-0.16	0.09	0.66
<b>9,10-DiHOME</b>	Lipid	Fatty Acid, Dihydroxy	-0.38	0.09	0.66
<b>isobutyrylglycine (C4)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.20	0.09	0.66
<b>methionine sulfoxide</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.15	0.09	0.66
<b>7-dehydro-cholesterol</b>	Lipid	Sterol	0.63	0.09	0.66
<b>4-imidazoleacetate</b>	Amino Acid	Histidine Metabolism	-0.46	0.09	0.66
<b>isovalerylglycine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.22	0.09	0.66
<b>betaine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.11	0.09	0.66
<b>TL18:2n6 (linoleic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.08	0.09	0.66

<b>1-arachidonoyl-GPC* (20:4)*</b>	Lipid	Lysolipid	0.16	0.10	0.66
<b>2-ethylhexanoic acid</b>	Xenobiotics	Chemical	-0.15	0.10	0.66
<b>TLdm16:0 (plasmalogen palmitic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.14	0.10	0.66
<b>1-linolenoylglycerophosphocholine (18:3n3)*</b>	Lipid	Lysolipid	0.22	0.10	0.66
<b>tauroolithocholate 3-sulfate</b>	Lipid	Secondary Bile Acid Metabolism	-0.58	0.10	0.66
<b>o-cresol sulfate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.97	0.10	0.66
<b>glucose</b>	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.10	0.10	0.66
<b>oleamide</b>	Lipid	Fatty Acid, Amide	0.31	0.10	0.66
<b>dimethylarginine (ADMA + SDMA)</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.06	0.10	0.66
<b>pyroglutamylglutamine</b>	Peptide	Dipeptide	0.29	0.10	0.66
<b>N-acetyl-aspartyl-glutamate (NAAG)</b>	Amino Acid	Glutamate Metabolism	-0.13	0.10	0.66
<b>phenylalanylleucine</b>	Peptide	Dipeptide	0.52	0.11	0.67
<b>2-hydroxy-3-methylvalerate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.17	0.11	0.67
<b>homostachydrine*</b>	Xenobiotics	Food Component/Plant	-0.21	0.11	0.69
<b>malonate (propanedioate)</b>	Lipid	Fatty Acid Synthesis	-0.26	0.11	0.69
<b>2-palmitoleoyl-GPC* (16:1)*</b>	Lipid	Lysolipid	0.31	0.12	0.71
<b>TL18:4n3 (stearidonic acid)</b>	Lipid	Mole % Total Fatty Acid	0.32	0.12	0.73
<b>TL18:1n9 (oleic acid)</b>	Lipid	Mole % Total Fatty Acid	0.06	0.12	0.73
<b>1,2,3-benzenetriol sulfate (2)</b>	Xenobiotics	Chemical	-0.75	0.12	0.73
<b>glycolithocholate sulfate*</b>	Lipid	Secondary Bile Acid Metabolism	-0.44	0.12	0.73
<b>N-acetylglutamate</b>	Amino Acid	Glutamate Metabolism	-0.41	0.13	0.73
<b>TLdm18:0 (plasmalogen stearic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.14	0.13	0.73
<b>TLTL (Total Total Lipid)</b>	Lipid	Quantitative Total Fatty Acid	0.13	0.13	0.73
<b>N-acetylglutamine</b>	Amino Acid	Glutamate Metabolism	-0.18	0.13	0.73
<b>stearidonate (18:4n3)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.20	0.13	0.73
<b>galactonate</b>	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.72	0.13	0.73
<b>gamma-glutamyltyrosine</b>	Peptide	Gamma-glutamyl Amino Acid	-0.11	0.13	0.73
<b>xylitol</b>	Carbohydrate	Pentose Metabolism	0.25	0.13	0.73
<b>tyrosine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.08	0.14	0.73
<b>4-guanidinobutanoate</b>	Amino Acid	Guanidino and Acetamido Metabolism	-0.49	0.14	0.74
<b>N-acetyltryptophan</b>	Amino Acid	Tryptophan Metabolism	0.17	0.14	0.74
<b>1-palmitoyl-GPC (16:0)</b>	Lipid	Lysolipid	0.12	0.14	0.74
<b>2-arachidonoyl-GPC* (20:4)*</b>	Lipid	Lysolipid	0.16	0.15	0.74

<b>3-methyl-2-oxobutyrate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.09	0.15	0.74
<b>N2,N5-diacetylornithine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.31	0.15	0.74
<b>alanine</b>	Amino Acid	Alanine and Aspartate Metabolism	0.07	0.15	0.74
<b>glycolate (hydroxyacetate)</b>	Xenobiotics	Chemical	-0.09	0.15	0.74
<b>uridine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.08	0.15	0.74
<b>xanthosine</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.17	0.15	0.74
<b>pregnen-diol disulfate*</b>	Lipid	Steroid	-0.23	0.15	0.75
<b>inositol 1-phosphate (I1P)</b>	Lipid	Inositol Metabolism	0.17	0.15	0.75
<b>N-acetyl glycine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	0.18	0.16	0.75
<b>2-linoleoyl-GPE* (18:2)*</b>	Lipid	Lysolipid	0.18	0.16	0.75
<b>stearoyl-linoleoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	-0.10	0.16	0.75
<b>stearate (18:0)</b>	Lipid	Long Chain Fatty Acid	0.07	0.16	0.75
<b>gamma-glutamylthreonine*</b>	Peptide	Gamma-glutamyl Amino Acid	-0.14	0.16	0.75
<b>homoarginine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.42	0.16	0.75
<b>O-sulfo-L-tyrosine</b>	Xenobiotics	Chemical	0.10	0.16	0.75
<b>2-palmitoyl-GPC* (16:0)*</b>	Lipid	Lysolipid	0.14	0.16	0.75
<b>N2-acetyllysine</b>	Amino Acid	Lysine Metabolism	-0.23	0.17	0.75
<b>16-hydroxypalmitate</b>	Lipid	Fatty Acid, Monohydroxy	-0.10	0.17	0.75
<b>gentisate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.63	0.17	0.75
<b>ribitol</b>	Carbohydrate	Pentose Metabolism	0.09	0.17	0.75
<b>stearoylcarnitine (C18)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.17	0.17	0.75
<b>TL14:1n5 (myristoleic acid)</b>	Lipid	Mole % Total Fatty Acid	0.24	0.17	0.75
<b>glycocholate sulfate*</b>	Lipid	Secondary Bile Acid Metabolism	-0.15	0.17	0.75
<b>N-acetyltaurine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.17	0.17	0.75
<b>gamma-CEHC</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.20	0.18	0.75
<b>homocitrulline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.18	0.18	0.75
<b>trans-urocanate</b>	Amino Acid	Histidine Metabolism	0.18	0.18	0.75
<b>1-palmitoleoyl-GPC* (16:1)*</b>	Lipid	Lysolipid	0.18	0.18	0.75
<b>sphingomyelin</b>	Lipid	Sphingolipid Metabolism	0.11	0.18	0.75
<b>4-androsten-3beta,17beta-diol monosulfate (2)</b>	Lipid	Steroid	-0.34	0.18	0.75
<b>proline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.08	0.18	0.75
<b>cysteine-glutathione disulfide</b>	Amino Acid	Glutathione Metabolism	-0.38	0.18	0.75

<b>1-docosahexaenoyl-GPC* (22:6)*</b>	Lipid	Lysolipid	0.17	0.18	0.76
<b>7-methylguanine</b>	Nucleotide	Purine Metabolism, Guanine containing	-0.08	0.19	0.76
<b>palmitoyl-oleoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	0.10	0.19	0.76
<b>hydroxybutyrylcarnitine*</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.25	0.19	0.76
<b>4-hydroxyphenylpyruvate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.18	0.19	0.76
<b>kynurenate</b>	Amino Acid	Tryptophan Metabolism	-0.14	0.19	0.76
<b>3-methylglutarylcarnitine (2)</b>	Amino Acid	Lysine Metabolism	0.22	0.19	0.76
<b>3-methoxytyramine sulfate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.16	0.19	0.76
<b>allo-isoleucine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.09	0.19	0.76
<b>tetradecanedioate (C14)</b>	Lipid	Fatty Acid, Dicarboxylate	-0.17	0.20	0.76
<b>TL18:0 (stearic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.05	0.20	0.76
<b>arginine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.10	0.20	0.76
<b>pipecolate</b>	Amino Acid	Lysine Metabolism	-0.19	0.20	0.76
<b>N-acetylcitrulline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.35	0.20	0.77
<b>phenylalanine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.05	0.20	0.77
<b>TLdm18:1n9 (plasmalogen oleic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.13	0.21	0.77
<b>7-HOCA</b>	Lipid	Sterol	0.13	0.21	0.77
<b>hydroquinone sulfate</b>	Xenobiotics	Drug	-0.37	0.21	0.77
<b>N-acetylaspartate (NAA)</b>	Amino Acid	Alanine and Aspartate Metabolism	-0.08	0.21	0.77
<b>N-acetylarginine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.15	0.21	0.77
<b>1-stearoylplasmeneylethanolamine *</b>	Lipid	Lysolipid	0.15	0.21	0.77
<b>cyclohexanebutanoic acid</b>	Xenobiotics	Chemical	-0.15	0.21	0.77
<b>pyroglutamine*</b>	Amino Acid	Glutamate Metabolism	-0.19	0.21	0.77
<b>cys-gly, oxidized</b>	Amino Acid	Glutathione Metabolism	0.24	0.22	0.77
<b>4-methyl-2-oxopentanoate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.08	0.22	0.77
<b>3beta,7beta-dihydroxy-5-cholestenoate</b>	Lipid	Sterol	-0.11	0.22	0.77
<b>1,6-anhydroglucose</b>	Xenobiotics	Food Component/Plant	-0.29	0.22	0.77
<b>arachidate (20:0)</b>	Lipid	Long Chain Fatty Acid	0.08	0.22	0.77
<b>hexadecanedioate (C16)</b>	Lipid	Fatty Acid, Dicarboxylate	-0.16	0.22	0.77
<b>5alpha-androstan-3beta,17beta-diol disulfate</b>	Lipid	Steroid	-0.33	0.22	0.77
<b>seryltyrosine</b>	Peptide	Dipeptide	0.31	0.22	0.77
<b>octadecanedioate (C18)</b>	Lipid	Fatty Acid, Dicarboxylate	-0.16	0.23	0.77

<b>4-hydroxyhippurate</b>	Xenobiotics	Benzoate Metabolism	-0.25	0.23	0.77
<b>dopamine sulfate (2)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.14	0.23	0.77
<b>docosahexaenoate (DHA; 22:6n3)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.14	0.23	0.77
<b>N-acetylthreonine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	0.12	0.23	0.77
<b>alpha-tocopherol</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.13	0.23	0.77
<b>N-methylpipecolate</b>	Xenobiotics	Chemical	-0.22	0.23	0.77
<b>beta-hydroxyisovaleroylcarnitine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.11	0.23	0.78
<b>prolylhydroxyproline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.16	0.23	0.78
<b>N-acetylcarnosine</b>	Peptide	Dipeptide Derivative	-0.09	0.24	0.78
<b>trimethylamine N-oxide</b>	Lipid	Phospholipid Metabolism	0.56	0.24	0.79
<b>aspartylphenylalanine</b>	Peptide	Dipeptide	0.28	0.24	0.79
<b>andro steroid monosulfate (1)*</b>	Lipid	Steroid	-0.32	0.25	0.80
<b>3-methylglutaconate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.18	0.25	0.80
<b>cysteine s-sulfate</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.09	0.25	0.80
<b>2-eicosatrienoyl-GPC* (20:3)*</b>	Lipid	Lysolipid	0.11	0.26	0.80
<b>asparagine</b>	Amino Acid	Alanine and Aspartate Metabolism	-0.05	0.26	0.80
<b>pregn steroid monosulfate*</b>	Lipid	Steroid	-0.18	0.26	0.80
<b>1-oleoyl-GPC (18:1)</b>	Lipid	Lysolipid	0.12	0.26	0.80
<b>TL16:1n7 (palmitoleic acid)</b>	Lipid	Mole % Total Fatty Acid	0.11	0.26	0.80
<b>TL24:1n9 (nervonic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.12	0.26	0.80
<b>quinat</b>	Xenobiotics	Food Component/Plant	0.59	0.26	0.80
<b>21-hydroxypregnenolone disulfate</b>	Lipid	Steroid	-0.19	0.26	0.80
<b>deoxycarnitine</b>	Lipid	Carnitine Metabolism	-0.06	0.26	0.80
<b>paraxanthine</b>	Xenobiotics	Xanthine Metabolism	-0.57	0.26	0.80
<b>1-methylnicotinamide</b>	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-0.32	0.26	0.80
<b>4-ethylphenyl sulfate</b>	Xenobiotics	Benzoate Metabolism	0.27	0.27	0.80
<b>inosine</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.35	0.27	0.80
<b>mannose</b>	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.08	0.27	0.80
<b>ethylmalonate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.13	0.27	0.80
<b>eicosapentaenoate (EPA; 20:5n3)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.18	0.27	0.80
<b>N6-succinyladenosine</b>	Nucleotide	Purine Metabolism, Adenine containing	0.09	0.27	0.80
<b>creatine</b>	Amino Acid	Creatine Metabolism	0.13	0.27	0.80



<b>1-pentadecanoylglycerol (1-monopentadecanoin)</b>	Lipid	Monoacylglycerol	0.15	0.27	0.80
<b>methyl-4-hydroxybenzoate sulfate</b>	Xenobiotics	Benzoate Metabolism	-0.48	0.27	0.80
<b>5,6-dihydrothymine</b>	Nucleotide	Pyrimidine Metabolism, Thymine containing	-0.09	0.28	0.80
<b>adrenate (22:4n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.10	0.28	0.80
<b>acetoacetate</b>	Lipid	Ketone Bodies	-0.17	0.28	0.80
<b>TL20:5n3 (eicosapentaenoic acid)</b>	Lipid	Mole % Total Fatty Acid	0.17	0.28	0.80
<b>1-eicosatrienoyl-GPC* (20:3)*</b>	Lipid	Lysolipid	0.12	0.28	0.80
<b>piperine</b>	Xenobiotics	Food Component/Plant	-0.24	0.28	0.80
<b>nonadecanoate (19:0)</b>	Lipid	Long Chain Fatty Acid	0.06	0.28	0.80
<b>5alpha-androstan-3alpha,17beta-diol disulfate</b>	Lipid	Steroid	-0.38	0.28	0.81
<b>glucarate 1,4-lactone</b>	Carbohydrate	Disaccharides and Oligosaccharides	-0.78	0.29	0.81
<b>TL22:5n3 (docosapentaenoic acid)</b>	Lipid	Mole % Total Fatty Acid	0.08	0.29	0.81
<b>TL20:1n9 (eicoasaenoic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.05	0.30	0.81
<b>ectoine</b>	Xenobiotics	Chemical	-0.29	0.30	0.81
<b>3-hydroxy-3-methylglutarate</b>	Lipid	Mevalonate Metabolism	0.08	0.30	0.81
<b>valine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.04	0.30	0.81
<b>sulfate*</b>	Xenobiotics	Chemical	0.04	0.30	0.81
<b>indoleacetate</b>	Amino Acid	Tryptophan Metabolism	0.14	0.30	0.81
<b>palmitoylcarnitine (C16)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.12	0.30	0.81
<b>cyclo(L-phe-L-pro)</b>	Peptide	Dipeptide	-0.23	0.31	0.81
<b>1-stearoyl-GPC (18:0)</b>	Lipid	Lysolipid	0.12	0.31	0.81
<b>fucose</b>	Carbohydrate	Pentose Metabolism	0.11	0.31	0.81
<b>N-acetylputrescine</b>	Amino Acid	Polyamine Metabolism	0.11	0.31	0.81
<b>cortisone</b>	Lipid	Steroid	-0.16	0.31	0.81
<b>12,13-DiHOME</b>	Lipid	Fatty Acid, Dihydroxy	-0.15	0.31	0.81
<b>oleoyl-linoleoyl-glycerophosphocholine (2)*</b>	Lipid	Lysolipid	0.08	0.31	0.81
<b>gamma-glutamylmethionine</b>	Peptide	Gamma-glutamyl Amino Acid	-0.11	0.31	0.81
<b>histidylphenylalanine</b>	Peptide	Dipeptide	0.31	0.31	0.81
<b>caffeine</b>	Xenobiotics	Xanthine Metabolism	-0.48	0.32	0.81
<b>ornithine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.08	0.32	0.81
<b>N-acetyl-1-methylhistidine*</b>	Amino Acid	Histidine Metabolism	-0.15	0.32	0.81
<b>7-methylurate</b>	Xenobiotics	Xanthine Metabolism	-0.49	0.32	0.81
<b>lactate</b>	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.06	0.32	0.81
<b>citrulline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.10	0.32	0.81

<b>leucylalanine</b>	Peptide	Dipeptide	0.26	0.32	0.81
<b>alpha-ketobutyrate</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.21	0.32	0.81
<b>arachidonate (20:4n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.06	0.32	0.81
<b>androsterone sulfate</b>	Lipid	Steroid	-0.27	0.32	0.81
<b>3-hydroxypyridine sulfate</b>	Xenobiotics	Chemical	0.31	0.32	0.81
<b>glutamate</b>	Amino Acid	Glutamate Metabolism	0.08	0.33	0.81
<b>lanosterol</b>	Lipid	Sterol	0.27	0.33	0.81
<b>2-aminooctanoate</b>	Lipid	Fatty Acid, Amino	0.14	0.33	0.82
<b>histidine</b>	Amino Acid	Histidine Metabolism	0.09	0.33	0.82
<b>N-acetylneuraminate</b>	Carbohydrate	Aminosugar Metabolism	0.11	0.34	0.82
<b>TL18:3n3 (a-linolenic acid)</b>	Lipid	Mole % Total Fatty Acid	0.07	0.34	0.82
<b>docosapentaenoate (n6 DPA; 22:5n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.08	0.34	0.82
<b>dehydroisoandrosterone sulfate (DHEA-S)</b>	Lipid	Steroid	-0.19	0.34	0.82
<b>1-palmitoylplasmeneylethanolamine*</b>	Lipid	Lysolipid	0.08	0.34	0.82
<b>1-docosapentaenoyl-GPC* (22:5n3)*</b>	Lipid	Lysolipid	0.11	0.34	0.82
<b>3-indoxyl sulfate</b>	Amino Acid	Tryptophan Metabolism	0.15	0.34	0.82
<b>desmosterol</b>	Lipid	Sterol	-0.17	0.35	0.82
<b>cholestanol</b>	Lipid	Sterol	-0.09	0.35	0.82
<b>pyridoxate</b>	Cofactors and Vitamins	Vitamin B6 Metabolism	0.19	0.35	0.82
<b>palmitoyl-arachidonoyl-glycerophosphocholine (2)*</b>	Lipid	Lysolipid	0.06	0.35	0.82
<b>10-undecenoate (11:1n1)</b>	Lipid	Medium Chain Fatty Acid	-0.10	0.35	0.83
<b>dodecanedioate (C12)</b>	Lipid	Fatty Acid, Dicarboxylate	-0.12	0.35	0.83
<b>3-hydroxyoctanoate</b>	Lipid	Fatty Acid, Monohydroxy	-0.11	0.35	0.83
<b>imidazole lactate</b>	Amino Acid	Histidine Metabolism	-0.09	0.36	0.83
<b>oxalate (ethanedioate)</b>	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	-0.16	0.36	0.83
<b>isoleucine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.04	0.36	0.83
<b>taurochenodeoxycholate</b>	Lipid	Primary Bile Acid Metabolism	-0.29	0.36	0.83
<b>N6-methyladenosine</b>	Nucleotide	Purine Metabolism, Adenine containing	0.10	0.36	0.83
<b>alpha-hydroxyisovalerate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.11	0.37	0.84
<b>stachydrine</b>	Xenobiotics	Food Component/Plant	0.29	0.37	0.84
<b>palmitoyl-arachidonoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	0.11	0.37	0.84
<b>5-hydroxyindoleacetate</b>	Amino Acid	Tryptophan Metabolism	0.09	0.37	0.84
<b>palmitate (16:0)</b>	Lipid	Long Chain Fatty Acid	0.05	0.37	0.84

<b>4-ureidobutyrate</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.14	0.37	0.84
<b>myristoylcarnitine</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.13	0.37	0.84
<b>eicosenoyl sphingomyelin*</b>	Lipid	Sphingolipid Metabolism	0.08	0.37	0.84
<b>myristoyl sphingomyelin*</b>	Lipid	Sphingolipid Metabolism	0.05	0.38	0.84
<b>ursodeoxycholate</b>	Lipid	Secondary Bile Acid Metabolism	0.37	0.38	0.84
<b>leucine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.04	0.38	0.84
<b>theophylline</b>	Xenobiotics	Xanthine Metabolism	-0.36	0.38	0.85
<b>serotonin (5HT)</b>	Amino Acid	Tryptophan Metabolism	0.23	0.39	0.85
<b>oleoylcarnitine (C18)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.11	0.39	0.85
<b>cis-4-decenoyl carnitine</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.09	0.39	0.85
<b>glycerophosphorylcholine (GPC)</b>	Lipid	Phospholipid Metabolism	0.06	0.39	0.85
<b>TL22:0 (behenic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.09	0.39	0.85
<b>maleate (cis-Butenedioate)</b>	Lipid	Fatty Acid, Dicarboxylate	0.13	0.39	0.85
<b>TL16:0 (palmitic acid)</b>	Lipid	Mole % Total Fatty Acid	0.03	0.39	0.85
<b>1-linoleoyl-GPE (18:2)*</b>	Lipid	Lysolipid	0.08	0.40	0.85
<b>acetylcarnitine (C2)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.08	0.40	0.85
<b>lathosterol</b>	Lipid	Sterol	0.15	0.41	0.85
<b>glycylproline</b>	Peptide	Dipeptide	0.22	0.41	0.85
<b>12-HETE</b>	Lipid	Eicosanoid	-0.23	0.41	0.85
<b>docosapentaenoate (DPA; 22:5n3)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.09	0.41	0.85
<b>serine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.05	0.41	0.85
<b>threonate</b>	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	-0.14	0.41	0.85
<b>mannitol</b>	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.27	0.41	0.85
<b>2-linoleoyl-GPC* (18:2)*</b>	Lipid	Lysolipid	0.09	0.41	0.85
<b>5-oxoproline</b>	Amino Acid	Glutathione Metabolism	-0.07	0.41	0.85
<b>theobromine</b>	Xenobiotics	Xanthine Metabolism	-0.27	0.41	0.85
<b>10-nonadecenoate (19:1n9)</b>	Lipid	Long Chain Fatty Acid	0.08	0.41	0.85
<b>cyclo(leu-pro)</b>	Peptide	Dipeptide	-0.15	0.41	0.85
<b>succinate</b>	Energy	TCA Cycle	-0.04	0.41	0.85
<b>quinolinate</b>	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.14	0.42	0.86
<b>methylsuccinate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.06	0.42	0.86
<b>pyroglutamylglycine</b>	Peptide	Dipeptide	0.19	0.42	0.86
<b>hydroxyproline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.10	0.42	0.86
<b>3-(3-hydroxyphenyl)propionate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.34	0.42	0.86

<b>urea</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.07	0.42	0.86
<b>TLdm18:1n7 (plasmalogen vaccenic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.17	0.43	0.86
<b>pregnenediol-3-glucuronide</b>	Lipid	Steroid	-0.27	0.43	0.86
<b>nicotinamide</b>	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.11	0.43	0.86
<b>sphinganine</b>	Lipid	Sphingolipid Metabolism	0.28	0.43	0.86
<b>myristoleoyl sphingomyelin*</b>	Lipid	Sphingolipid Metabolism	-0.10	0.43	0.86
<b>caprylate (8:0)</b>	Lipid	Medium Chain Fatty Acid	-0.05	0.43	0.86
<b>urate</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.05	0.44	0.86
<b>pseudouridine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.04	0.44	0.86
<b>dimethyl sulfone</b>	Xenobiotics	Chemical	0.26	0.44	0.86
<b>palmitoleoyl sphingomyelin*</b>	Lipid	Sphingolipid Metabolism	-0.04	0.44	0.86
<b>3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)</b>	Lipid	Fatty Acid, Dicarboxylate	0.30	0.44	0.86
<b>1-methylguanosine</b>	Nucleotide	Purine Metabolism, Guanine containing	0.04	0.44	0.86
<b>N-acetylphenylalanine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.09	0.44	0.86
<b>1-palmitoylglycerophosphate</b>	Lipid	Lysolipid	0.13	0.45	0.86
<b>2-hydroxystearate</b>	Lipid	Fatty Acid, Monohydroxy	-0.04	0.45	0.86
<b>4-androsten-3alpha,17alpha-diol monosulfate (3)</b>	Lipid	Steroid	-0.20	0.45	0.86
<b>1,7-dimethylurate</b>	Xenobiotics	Xanthine Metabolism	-0.32	0.45	0.86
<b>3-methyl-2-oxovalerate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.05	0.45	0.87
<b>kynurenine</b>	Amino Acid	Tryptophan Metabolism	0.05	0.46	0.87
<b>tartarate</b>	Xenobiotics	Food Component/Plant	-0.23	0.46	0.87
<b>N-palmitoyl glycine</b>	Lipid	Fatty Acid Metabolism(Acyl Glycine)	-0.10	0.46	0.87
<b>beta-tocopherol</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.17	0.46	0.87
<b>N-acetyltyrosine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.08	0.46	0.87
<b>4-vinylphenol sulfate</b>	Xenobiotics	Benzoate Metabolism	-0.23	0.46	0.87
<b>glycolithocholate</b>	Lipid	Secondary Bile Acid Metabolism	-0.32	0.46	0.87
<b>17-methylstearate</b>	Lipid	Fatty Acid, Branched	0.08	0.46	0.87
<b>ribonate (ribonolactone)</b>	Carbohydrate	Pentose Metabolism	-0.07	0.46	0.87
<b>erythritol</b>	Xenobiotics	Food Component/Plant	0.10	0.47	0.87
<b>phenylalanylphenylalanine</b>	Peptide	Dipeptide	0.11	0.47	0.87
<b>stearoyl-linoleoyl-glycerophosphoethanolamine (1)*</b>	Lipid	Lysolipid	0.10	0.47	0.87
<b>4-acetamidobutanoate</b>	Amino Acid	Polyamine Metabolism	0.06	0.47	0.87

<b>pentadecanoate (15:0)</b>	Lipid	Long Chain Fatty Acid	0.05	0.47	0.87
<b>bilirubin</b>	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-0.21	0.48	0.87
<b>2-aminoheptanoate</b>	Lipid	Fatty Acid, Amino	0.07	0.48	0.87
<b>4-androsten-3beta,17beta-diol disulfate (1)</b>	Lipid	Steroid	-0.16	0.48	0.87
<b>taurine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.07	0.48	0.88
<b>2-hydroxyoctanoate</b>	Lipid	Fatty Acid, Monohydroxy	0.08	0.48	0.88
<b>4-androsten-3alpha,17alpha-diol monosulfate (2)</b>	Lipid	Steroid	-0.17	0.49	0.88
<b>5-methylthioadenosine (MTA)</b>	Amino Acid	Polyamine Metabolism	0.23	0.49	0.88
<b>tiglyl carnitine (C5)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.08	0.49	0.88
<b>tyrosylglutamate</b>	Peptide	Dipeptide	0.19	0.49	0.88
<b>5alpha-pregnan-3beta,20alpha-diol disulfate</b>	Lipid	Steroid	-0.15	0.49	0.88
<b>2-linolenoylglycerophosphocholine (18:3n3)*</b>	Lipid	Lysolipid	-0.23	0.49	0.88
<b>pantothenate (Vitamin B5)</b>	Cofactors and Vitamins	Pantothenate and CoA Metabolism	0.08	0.49	0.88
<b>dopamine sulfate (1)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.12	0.50	0.88
<b>pyrraline</b>	Xenobiotics	Food Component/Plant	0.17	0.50	0.88
<b>TL22:4n6 (adrenic acid)</b>	Lipid	Mole % Total Fatty Acid	0.06	0.50	0.88
<b>tartronate (hydroxymalonate)</b>	Xenobiotics	Bacterial/Fungal	-0.11	0.50	0.88
<b>1,3-dimethylurate</b>	Xenobiotics	Xanthine Metabolism	-0.30	0.50	0.89
<b>alpha-hydroxyisocaproate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.06	0.50	0.89
<b>5-dodecenoate (12:1n7)</b>	Lipid	Medium Chain Fatty Acid	-0.08	0.51	0.89
<b>erythronate*</b>	Carbohydrate	Aminosugar Metabolism	0.04	0.51	0.89
<b>TL15:0 (pentadecanoic acid)</b>	Lipid	Mole % Total Fatty Acid	0.03	0.52	0.90
<b>N-acetylkynurenine (2)</b>	Amino Acid	Tryptophan Metabolism	-0.21	0.52	0.90
<b>2-aminophenol sulfate</b>	Xenobiotics	Chemical	0.19	0.52	0.90
<b>2-pyrrolidinone</b>	Xenobiotics	Chemical	-0.12	0.52	0.90
<b>homovanillate (HVA)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.08	0.52	0.90
<b>malate</b>	Energy	TCA Cycle	-0.05	0.52	0.90
<b>glycylvaline</b>	Peptide	Dipeptide	0.26	0.53	0.90
<b>stearoyl-arachidonoylglycerophosphoinositol (1)*</b>	Lipid	Lysolipid	0.05	0.53	0.90
<b>phenyllactate (PLA)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.05	0.53	0.90
<b>TL22:1n9 (erucic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.14	0.54	0.91
<b>squalene</b>	Lipid	Sterol	0.19	0.54	0.91
<b>TL22:6n3 (docosahexaenoic acid)</b>	Lipid	Mole % Total Fatty Acid	0.06	0.54	0.91

<b>1-eicosenoylglycerophosphocholine (20:1n9)*</b>	Lipid	Lysolipid	0.09	0.54	0.91
<b>myristoleate (14:1n5)</b>	Lipid	Long Chain Fatty Acid	-0.16	0.54	0.91
<b>leucylglycine</b>	Peptide	Dipeptide	0.22	0.54	0.91
<b>stearoyl-arachidonoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	-0.13	0.54	0.91
<b>glycerol 3-phosphate (G3P)</b>	Lipid	Glycerolipid Metabolism	-0.15	0.54	0.91
<b>glucuronate</b>	Carbohydrate	Aminosugar Metabolism	0.06	0.54	0.91
<b>3-hydroxydecanoate</b>	Lipid	Fatty Acid, Monohydroxy	-0.06	0.55	0.91
<b>3-hydroxyhippurate</b>	Xenobiotics	Benzoate Metabolism	-0.22	0.55	0.91
<b>5,6-dihydrouracil</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.05	0.55	0.91
<b>N-acetylisoleucine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.09	0.55	0.91
<b>HWESASXX*</b>	Peptide	Polypeptide	-0.14	0.55	0.91
<b>octanoylcarnitine (C8)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.05	0.56	0.91
<b>1,3,7-trimethylurate</b>	Xenobiotics	Xanthine Metabolism	-0.21	0.56	0.91
<b>indole-3-carboxylic acid</b>	Amino Acid	Tryptophan Metabolism	0.04	0.56	0.91
<b>2-stearoyl-GPC* (18:0)*</b>	Lipid	Lysolipid	0.08	0.56	0.91
<b>cortisol</b>	Lipid	Steroid	-0.08	0.56	0.91
<b>vanillylmandelate (VMA)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.07	0.56	0.91
<b>tryptophan</b>	Amino Acid	Tryptophan Metabolism	-0.03	0.56	0.91
<b>1-palmitoyl-GPI* (16:0)*</b>	Lipid	Lysolipid	0.09	0.56	0.91
<b>S-adenosylhomocysteine (SAH)</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.08	0.57	0.91
<b>allantoin</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.09	0.57	0.91
<b>prolylglycine</b>	Peptide	Dipeptide	-0.11	0.57	0.91
<b>palmitoyl-oleoyl-glycerophosphoglycerol (2)*</b>	Lipid	Lysolipid	-0.20	0.57	0.91
<b>margarate (17:0)</b>	Lipid	Long Chain Fatty Acid	0.05	0.58	0.92
<b>eicosanodioate</b>	Lipid	Fatty Acid, Dicarboxylate	-0.08	0.58	0.92
<b>adenine</b>	Nucleotide	Purine Metabolism, Adenine containing	-0.07	0.58	0.92
<b>I-urobilinogen</b>	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	0.25	0.58	0.92
<b>cholate</b>	Lipid	Primary Bile Acid Metabolism	0.22	0.59	0.92
<b>p-cresol sulfate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.16	0.59	0.92
<b>arabonate</b>	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.05	0.59	0.92
<b>beta-sitosterol</b>	Lipid	Sterol	0.07	0.59	0.92
<b>gamma-glutamylphenylalanine</b>	Peptide	Gamma-glutamyl Amino Acid	-0.03	0.59	0.92

<b>isovalerate (C5)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.05	0.59	0.92
<b>phenol sulfate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.16	0.59	0.92
<b>choline</b>	Lipid	Phospholipid Metabolism	0.03	0.60	0.92
<b>oleic ethanolamide</b>	Lipid	Endocannabinoid	-0.05	0.60	0.93
<b>levulinate (4-oxovalerate)</b>	Xenobiotics	Food Component/Plant	-0.06	0.60	0.93
<b>3-hydroxymyristate</b>	Lipid	Fatty Acid, Monohydroxy	-0.05	0.60	0.93
<b>phenylalanylglutamate</b>	Peptide	Dipeptide	0.27	0.61	0.93
<b>palmitoyl-linoleoyl-glycerophosphoinositol (1)*</b>	Lipid	Lysolipid	0.11	0.61	0.93
<b>cystine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.03	0.61	0.93
<b>hypoxanthine</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.10	0.61	0.93
<b>2-hydroxypalmitate</b>	Lipid	Fatty Acid, Monohydroxy	-0.03	0.61	0.93
<b>TL20:3n6 (di-homo-g-linoleic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.03	0.61	0.93
<b>1,5-anhydroglucitol (1,5-AG)</b>	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	-0.08	0.62	0.93
<b>1-methylimidazoleacetate</b>	Amino Acid	Histidine Metabolism	-0.09	0.62	0.93
<b>salicylate</b>	Xenobiotics	Drug	-0.22	0.62	0.93
<b>1,2-propanediol</b>	Xenobiotics	Chemical	0.12	0.62	0.93
<b>saccharin</b>	Xenobiotics	Food Component/Plant	0.31	0.62	0.93
<b>phenylalanylserine</b>	Peptide	Dipeptide	-0.18	0.62	0.93
<b>1-linoleoyl-GPC (18:2)</b>	Lipid	Lysolipid	0.04	0.62	0.93
<b>aspartate</b>	Amino Acid	Alanine and Aspartate Metabolism	0.05	0.62	0.93
<b>N-acetyl-beta-alanine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.04	0.62	0.93
<b>2-methylbutyrylcarnitine (C5)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.04	0.62	0.93
<b>cyclo(pro-pro)</b>	Peptide	Dipeptide	0.06	0.63	0.93
<b>TL20:4n3 (eicosatetranoic acid)</b>	Lipid	Mole % Total Fatty Acid	0.06	0.63	0.93
<b>docosadienoate (22:2n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.04	0.63	0.93
<b>5alpha-androstan-3beta,17alpha-diol disulfate</b>	Lipid	Steroid	-0.15	0.63	0.93
<b>gamma-glutamyltryptophan</b>	Peptide	Gamma-glutamyl Amino Acid	-0.04	0.63	0.93
<b>phosphate</b>	Energy	Oxidative Phosphorylation	-0.02	0.63	0.93
<b>guanidinoacetate</b>	Amino Acid	Creatine Metabolism	-0.05	0.64	0.93
<b>3-methoxycatechol sulfate (1)</b>	Xenobiotics	Benzoate Metabolism	-0.18	0.64	0.93
<b>gamma-glutamylhistidine</b>	Peptide	Gamma-glutamyl Amino Acid	-0.11	0.64	0.93
<b>phenylacetylglutamine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.08	0.64	0.93
<b>vaccenate (18:1n7)</b>	Lipid	Long Chain Fatty Acid	-0.04	0.64	0.93

<b>C-glycosyltryptophan</b>	Amino Acid	Tryptophan Metabolism	0.02	0.65	0.93
<b>cholesterol</b>	Lipid	Sterol	-0.03	0.65	0.93
<b>taurodeoxycholate</b>	Lipid	Secondary Bile Acid Metabolism	-0.22	0.65	0.93
<b>2-piperidinone</b>	Xenobiotics	Food Component/Plant	0.13	0.65	0.93
<b>cinnamoylglycine</b>	Xenobiotics	Food Component/Plant	0.24	0.65	0.93
<b>4-allylphenol sulfate</b>	Xenobiotics	Food Component/Plant	0.12	0.65	0.93
<b>scyllo-inositol</b>	Lipid	Inositol Metabolism	-0.08	0.66	0.93
<b>stigmasterol</b>	Lipid	Sterol	-0.09	0.66	0.93
<b>3-[3-(sulfooxy)phenyl]propanoic acid</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.22	0.66	0.93
<b>2-methylmalonyl carnitine</b>	Lipid	Fatty Acid Synthesis	-0.04	0.66	0.93
<b>cyclo(gly-pro)</b>	Peptide	Dipeptide	0.07	0.66	0.93
<b>glycerol</b>	Lipid	Glycerolipid Metabolism	0.04	0.66	0.93
<b>N-acetyl-3-methylhistidine*</b>	Amino Acid	Histidine Metabolism	-0.13	0.66	0.93
<b>guanosine</b>	Nucleotide	Purine Metabolism, Guanine containing	-0.16	0.66	0.93
<b>N-methylproline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.12	0.66	0.93
<b>gamma-glutamylalanine</b>	Peptide	Gamma-glutamyl Amino Acid	0.04	0.66	0.93
<b>1-stearoyl-GPI (18:0)</b>	Lipid	Lysolipid	-0.04	0.67	0.93
<b>myristate (14:0)</b>	Lipid	Long Chain Fatty Acid	0.04	0.67	0.93
<b>hippurate</b>	Xenobiotics	Benzoate Metabolism	0.10	0.67	0.93
<b>1-stearoylglycerol (18:0)</b>	Lipid	Monoacylglycerol	0.13	0.67	0.93
<b>arabitol</b>	Carbohydrate	Pentose Metabolism	0.04	0.67	0.93
<b>glycocholate</b>	Lipid	Primary Bile Acid Metabolism	0.12	0.68	0.93
<b>isoleucylglycine</b>	Peptide	Dipeptide	0.10	0.68	0.93
<b>O-methylcatechol sulfate</b>	Xenobiotics	Benzoate Metabolism	0.09	0.68	0.93
<b>dimethylglycine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.04	0.68	0.93
<b>1-arachidonoyl-GPI* (20:4)*</b>	Lipid	Lysolipid	0.03	0.68	0.93
<b>thyroxine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.12	0.68	0.93
<b>4-androsten-3beta,17beta-diol monosulfate (1)</b>	Lipid	Steroid	-0.09	0.69	0.93
<b>hypotaurine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.09	0.69	0.93
<b>methylpalmitate (15 or 2)</b>	Lipid	Fatty Acid, Branched	0.04	0.69	0.93
<b>hydantoin-5-propionic acid</b>	Amino Acid	Histidine Metabolism	0.10	0.69	0.93
<b>dihomolinolenate (20:3n3 or 3n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.02	0.70	0.94
<b>1-arachidoyl-GPC (20:0)</b>	Lipid	Lysolipid	0.13	0.70	0.94
<b>2-hydroxybutyrate (AHB)</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.04	0.70	0.94
<b>tyramine O-sulfate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.11	0.70	0.94



<b>pelargonate (9:0)</b>	Lipid	Medium Chain Fatty Acid	-0.02	0.71	0.94
<b>valylarginine</b>	Peptide	Dipeptide	0.10	0.71	0.94
<b>histidyltryptophan</b>	Peptide	Dipeptide	-0.08	0.71	0.94
<b>4-hydroxychlorothalonil</b>	Xenobiotics	Chemical	0.06	0.71	0.94
<b>propionylcarnitine (C3)</b>	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.03	0.71	0.94
<b>palmitoyl-linoleoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	0.03	0.71	0.94
<b>glycerate</b>	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.03	0.71	0.94
<b>5-methyluridine (ribothymidine)</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.02	0.71	0.94
<b>5-HETE</b>	Lipid	Eicosanoid	0.07	0.72	0.94
<b>N2,N2-dimethylguanosine</b>	Nucleotide	Purine Metabolism, Guanine containing	0.02	0.72	0.94
<b>2-oleoyl-GPC* (18:1)*</b>	Lipid	Lysolipid	0.04	0.72	0.94
<b>indolelactate</b>	Amino Acid	Tryptophan Metabolism	0.03	0.72	0.94
<b>TL20:0 (arachidic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.03	0.72	0.94
<b>3-hydroxyisobutyrate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.04	0.72	0.94
<b>phenylalanyltryptophan</b>	Peptide	Dipeptide	0.06	0.72	0.94
<b>ADSGEGDFXAEGGGVR*</b>	Peptide	Fibrinogen Cleavage Peptide	0.04	0.72	0.94
<b>4-methylcatechol sulfate</b>	Xenobiotics	Benzoate Metabolism	-0.09	0.72	0.94
<b>3,7-dimethylurate</b>	Xenobiotics	Xanthine Metabolism	-0.12	0.72	0.94
<b>4-hydroxybenzoate</b>	Xenobiotics	Benzoate Metabolism	0.16	0.72	0.94
<b>TL20:2n6 (eicosadienoic acid)</b>	Lipid	Mole % Total Fatty Acid	0.03	0.73	0.94
<b>fumarate</b>	Energy	TCA Cycle	-0.03	0.73	0.95
<b>2'-deoxyuridine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.05	0.74	0.95
<b>linoleoylcarnitine*</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.05	0.74	0.95
<b>isobutyrylcarnitine (C4)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.04	0.74	0.95
<b>trigonelline (N'-methylnicotinate)</b>	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-0.08	0.75	0.95
<b>chenodeoxycholate</b>	Lipid	Primary Bile Acid Metabolism	0.09	0.75	0.95
<b>phenylcarnitine*</b>	Xenobiotics	Chemical	0.11	0.75	0.95
<b>3-methylxanthine</b>	Xenobiotics	Xanthine Metabolism	0.11	0.75	0.95
<b>N-formylmethionine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.02	0.75	0.95
<b>serylalanine</b>	Peptide	Dipeptide	0.05	0.75	0.95
<b>sphingosine 1-phosphate</b>	Lipid	Sphingolipid Metabolism	-0.02	0.76	0.95
<b>campesterol</b>	Lipid	Sterol	0.05	0.76	0.95
<b>catechol sulfate</b>	Xenobiotics	Benzoate Metabolism	-0.07	0.76	0.95
<b>3-hydroxylaurate</b>	Lipid	Fatty Acid, Monohydroxy	-0.03	0.76	0.95
<b>oleate (18:1n9)</b>	Lipid	Long Chain Fatty Acid	-0.03	0.76	0.95

<b>palmitoyl-palmitoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	0.04	0.76	0.95
<b>adenosine 3',5'-cyclic monophosphate (cAMP)</b>	Nucleotide	Purine Metabolism, Adenine containing	-0.07	0.76	0.95
<b>5alpha-pregnan-3beta,20alpha-diol monosulfate (2)</b>	Lipid	Steroid	-0.11	0.76	0.95
<b>1-eicosadienoyl-GPC* (20:2)*</b>	Lipid	Lysolipid	-0.04	0.77	0.95
<b>N-acetylalanine</b>	Amino Acid	Alanine and Aspartate Metabolism	0.01	0.77	0.95
<b>stearoyl-arachidonoyl-glycerophosphocholine (2)*</b>	Lipid	Lysolipid	-0.02	0.77	0.95
<b>carnitine</b>	Lipid	Carnitine Metabolism	-0.01	0.77	0.95
<b>pyroglutamylvaline</b>	Peptide	Dipeptide	0.03	0.77	0.95
<b>2-hydroxydecanoate</b>	Lipid	Fatty Acid, Monohydroxy	0.04	0.78	0.95
<b>pregnenolone sulfate</b>	Lipid	Steroid	-0.06	0.78	0.95
<b>salicyluric glucuronide*</b>	Xenobiotics	Drug	0.16	0.78	0.95
<b>TL22:5n6 (osbond acid)</b>	Lipid	Mole % Total Fatty Acid	0.03	0.78	0.95
<b>laurylcarnitine (C12)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.03	0.79	0.95
<b>N1-Methyl-2-pyridone-5-carboxamide</b>	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.04	0.79	0.95
<b>2-stearoylglycerophosphoinositol*</b>	Lipid	Lysolipid	-0.05	0.79	0.95
<b>cysteine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.03	0.79	0.95
<b>eicosenoate (20:1n9 or 1n11)</b>	Lipid	Long Chain Fatty Acid	0.03	0.79	0.95
<b>oleoyl sphingomyelin</b>	Lipid	Sphingolipid Metabolism	0.02	0.79	0.95
<b>phenylacetate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.04	0.79	0.95
<b>N-acetylalliin</b>	Xenobiotics	Food Component/Plant	0.11	0.79	0.95
<b>1-methylurate</b>	Xenobiotics	Xanthine Metabolism	-0.07	0.79	0.95
<b>3-ureidopropionate</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.03	0.79	0.95
<b>N-acetylvaline</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.01	0.80	0.95
<b>erucate (22:1n9)</b>	Lipid	Long Chain Fatty Acid	0.03	0.80	0.95
<b>isovalerylcarnitine (C5)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.03	0.80	0.95
<b>taurocholate</b>	Lipid	Primary Bile Acid Metabolism	-0.10	0.80	0.95
<b>dihydroorotate</b>	Nucleotide	Pyrimidine Metabolism, Orotate containing	0.06	0.80	0.96
<b>gamma-glutamylisoleucine*</b>	Peptide	Gamma-glutamyl Amino Acid	0.02	0.80	0.96
<b>gamma-glutamylglutamate</b>	Peptide	Gamma-glutamyl Amino Acid	0.04	0.81	0.96
<b>aspartylleucine</b>	Peptide	Dipeptide	0.04	0.81	0.96
<b>decanoylcarnitine (C10)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.02	0.82	0.97
<b>hexanoylcarnitine (C6)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.02	0.82	0.97
<b>2-hydroxyisobutyrate</b>	Xenobiotics	Chemical	0.02	0.82	0.97

<b>1-arachidonoyl glycerophosphate</b>	Lipid	Lysolipid	0.03	0.82	0.97
<b>tyrosylglutamine</b>	Peptide	Dipeptide	0.04	0.84	0.97
<b>gamma-tocopherol</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.03	0.84	0.97
<b>thymol sulfate</b>	Xenobiotics	Food Component/Plant	0.09	0.84	0.97
<b>N3-methyluridine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.03	0.84	0.97
<b>glycodeoxycholate</b>	Lipid	Secondary Bile Acid Metabolism	0.09	0.84	0.97
<b>13-methylmyristic acid</b>	Lipid	Fatty Acid, Branched	0.02	0.84	0.97
<b>2,3-dihydroxyisovalerate</b>	Xenobiotics	Food Component/Plant	0.07	0.84	0.97
<b>3-methoxycatechol sulfate (2)</b>	Xenobiotics	Benzoate Metabolism	-0.06	0.85	0.97
<b>tryptophylglutamate</b>	Peptide	Dipeptide	0.08	0.85	0.97
<b>glycine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.02	0.85	0.97
<b>fructose</b>	Carbohydrate	Fructose, Mannose and Galactose Metabolism	-0.02	0.85	0.97
<b>threitol</b>	Carbohydrate	Pentose Metabolism	0.02	0.85	0.97
<b>1-docosapentaenoyl-GPC* (22:5n6)*</b>	Lipid	Lysolipid	-0.06	0.85	0.97
<b>2-hydroxyhippurate (salicylurate)</b>	Xenobiotics	Benzoate Metabolism	-0.08	0.85	0.97
<b>glycylglycine</b>	Peptide	Dipeptide	-0.09	0.85	0.97
<b>epiandrosterone sulfate</b>	Lipid	Steroid	-0.05	0.85	0.97
<b>threonylphenylalanine</b>	Peptide	Dipeptide	0.08	0.85	0.97
<b>alpha-glutamyltyrosine</b>	Peptide	Dipeptide	0.06	0.85	0.97
<b>glycochenodeoxycholate</b>	Lipid	Primary Bile Acid Metabolism	-0.05	0.85	0.97
<b>imidazole propionate</b>	Amino Acid	Histidine Metabolism	-0.04	0.86	0.98
<b>serylleucine</b>	Peptide	Dipeptide	-0.07	0.86	0.98
<b>10-heptadecenoate (17:1n7)</b>	Lipid	Long Chain Fatty Acid	0.02	0.86	0.98
<b>glycoursodeoxycholate</b>	Lipid	Secondary Bile Acid Metabolism	-0.06	0.87	0.98
<b>TL20:4n6 (arachidonic acid)</b>	Lipid	Mole % Total Fatty Acid	0.01	0.87	0.98
<b>1-methylhistidine</b>	Amino Acid	Histidine Metabolism	-0.02	0.88	0.98
<b>N-acetylhistidine</b>	Amino Acid	Histidine Metabolism	0.03	0.88	0.98
<b>tryptophan betaine</b>	Amino Acid	Tryptophan Metabolism	-0.04	0.88	0.98
<b>valerylcarnitine (C5)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.06	0.88	0.98
<b>ribose</b>	Carbohydrate	Pentose Metabolism	0.03	0.88	0.98
<b>myo-inositol</b>	Lipid	Inositol Metabolism	0.01	0.89	0.98
<b>stearoyl-linoleoyl-glycerophosphocholine (2)*</b>	Lipid	Lysolipid	0.01	0.89	0.98
<b>gamma-glutamylleucine</b>	Peptide	Gamma-glutamyl Amino Acid	-0.01	0.89	0.98
<b>3-hydroxy-2-ethylpropionate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.01	0.89	0.98
<b>cis-Cyclo[L-ala-L-Pro]</b>	Peptide	Dipeptide	0.01	0.89	0.98

<b>N6-carbamoylthreonyladenosine</b>	Nucleotide	Purine Metabolism, Adenine containing	0.01	0.89	0.98
<b>N-6-trimethyllysine</b>	Amino Acid	Lysine Metabolism	-0.02	0.90	0.98
<b>N-acetylmethionine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.02	0.90	0.98
<b>5-acetylamino-6-amino-3-methyluracil</b>	Xenobiotics	Xanthine Metabolism	0.06	0.90	0.98
<b>3-phenylpropionate (hydrocinnamate)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.04	0.90	0.98
<b>7-methylxanthine</b>	Xenobiotics	Xanthine Metabolism	-0.04	0.90	0.98
<b>1-heptadecanoyl-GPC (17:0)</b>	Lipid	Lysolipid	0.02	0.90	0.98
<b>betonicine</b>	Xenobiotics	Food Component/Plant	0.07	0.90	0.98
<b>bilirubin (E,E)*</b>	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-0.02	0.91	0.98
<b>13-HODE + 9-HODE</b>	Lipid	Fatty Acid, Monohydroxy	0.02	0.91	0.98
<b>glutarate (pentanedioate)</b>	Amino Acid	Lysine Metabolism	-0.02	0.91	0.98
<b>glycylphenylalanine</b>	Peptide	Dipeptide	0.03	0.91	0.98
<b>laurate (12:0)</b>	Lipid	Medium Chain Fatty Acid	-0.01	0.91	0.98
<b>maltose</b>	Carbohydrate	Glycogen Metabolism	0.03	0.91	0.98
<b>N-oleoyltaurine</b>	Lipid	Endocannabinoid	-0.03	0.91	0.98
<b>ergothioneine</b>	Xenobiotics	Food Component/Plant	0.02	0.91	0.98
<b>delta-tocopherol</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.03	0.92	0.98
<b>caprate (10:0)</b>	Lipid	Medium Chain Fatty Acid	0.01	0.92	0.98
<b>2-arachidonoylglycerophosphoinositol*</b>	Lipid	Lysolipid	-0.02	0.92	0.98
<b>xanthine</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.01	0.92	0.98
<b>1-oleoyl-GPI (18:1)*</b>	Lipid	Lysolipid	0.01	0.92	0.98
<b>acisoga</b>	Amino Acid	Polyamine Metabolism	0.01	0.92	0.98
<b>2-aminoadipate</b>	Amino Acid	Lysine Metabolism	0.01	0.92	0.98
<b>1-oleoylplasmylethanolamine*</b>	Lipid	Lysolipid	0.01	0.92	0.98
<b>deoxycholate</b>	Lipid	Secondary Bile Acid Metabolism	0.02	0.92	0.98
<b>pyridoxal</b>	Cofactors and Vitamins	Vitamin B6 Metabolism	-0.04	0.92	0.98
<b>linoleate (18:2n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-0.01	0.94	0.99
<b>N-(2-furoyl)glycine</b>	Xenobiotics	Food Component/Plant	-0.01	0.94	0.99
<b>docosatrienoate (22:3n3)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-0.01	0.94	0.99
<b>glutaroylcarnitine (C5)</b>	Amino Acid	Lysine Metabolism	0.01	0.94	0.99
<b>TL18:1n7 (avaccenic acid)</b>	Lipid	Mole % Total Fatty Acid	0.003	0.94	0.99
<b>succinylcarnitine (C4)</b>	Energy	TCA Cycle	-0.01	0.94	0.99
<b>1-palmitoleoyl-GPI* (16:1)*</b>	Lipid	Lysolipid	0.03	0.94	0.99

<b>palmitoyl sphingomyelin</b>	Lipid	Sphingolipid Metabolism	0.003	0.95	0.99
<b>gamma-glutamyllysine</b>	Peptide	Gamma-glutamyl Amino Acid	-0.01	0.95	0.99
<b>1-linoleoyl-GPI* (18:2)*</b>	Lipid	Lysolipid	-0.01	0.95	0.99
<b>3-methylglutaryl carnitine (1)</b>	Amino Acid	Lysine Metabolism	0.01	0.95	0.99
<b>N-acetylserine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	0.003	0.96	0.99
<b>3-methylhistidine</b>	Amino Acid	Histidine Metabolism	0.01	0.96	0.99
<b>gamma-glutamyl-2-aminobutyrate</b>	Peptide	Gamma-glutamyl Amino Acid	0.01	0.96	0.99
<b>gamma-glutamylvaline</b>	Peptide	Gamma-glutamyl Amino Acid	0.003	0.96	0.99
<b>DSGEGDFXAEGGGVR*</b>	Peptide	Fibrinogen Cleavage Peptide	-0.01	0.96	0.99
<b>dihomolinoleate (20:2n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.004	0.97	0.99
<b>TL24:0 (lignoceric acid)</b>	Lipid	Mole % Total Fatty Acid	0.01	0.97	0.99
<b>3-(4-hydroxyphenyl)lactate (HPLA)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.003	0.97	0.99
<b>p-cresol-glucuronide*</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.02	0.97	0.99
<b>1-methyladenosine</b>	Nucleotide	Purine Metabolism, Adenine containing	-0.002	0.97	0.99
<b>5alpha-androstan-3alpha,17beta-diol monosulfate (1)</b>	Lipid	Steroid	0.01	0.97	0.99
<b>xylose</b>	Carbohydrate	Pentose Metabolism	0.01	0.97	0.99
<b>linolenate (18:3n3 or 3n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-0.004	0.97	0.99
<b>creatinine</b>	Amino Acid	Creatine Metabolism	-0.002	0.97	0.99
<b>adenosine</b>	Nucleotide	Purine Metabolism, Adenine containing	-0.01	0.97	0.99
<b>xylonate</b>	Carbohydrate	Pentose Metabolism	-0.01	0.97	0.99
<b>1-methylxanthine</b>	Xenobiotics	Xanthine Metabolism	-0.01	0.97	0.99
<b>lysine</b>	Amino Acid	Lysine Metabolism	0.002	0.97	0.99
<b>coprostanol</b>	Lipid	Sterol	-0.01	0.97	0.99
<b>palmitoleate (16:1n7)</b>	Lipid	Long Chain Fatty Acid	-0.004	0.98	0.99
<b>beta-hydroxyisovalerate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.003	0.98	0.99
<b>oleoyl-linoleoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	-0.001	0.99	0.99
<b>6-oxopiperidine-2-carboxylic acid</b>	Xenobiotics	Drug	0.001	0.99	0.99
<b>palmitoyl ethanolamide</b>	Lipid	Endocannabinoid	-0.001	0.99	0.99
<b>etiocholanolone glucuronide</b>	Lipid	Steroid	-0.004	0.99	0.99
<b>myristoleoyl carnitine*</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.002	0.99	0.99
<b>sorbitol</b>	Carbohydrate	Fructose, Mannose and Galactose Metabolism	-0.001	1.00	1.00
<b>palmitoyl-palmitoyl-glycerophosphocholine (2)*</b>	Lipid	Lysolipid	0.0003	0.97	1.00

\*Covariates: age, sex, diabetes, hypertension, BMI, and liver fibrosis stage

TCA = tricarboxylic acid cycle; GPE = Glycerophosphoethanolamine; GPC = Glycerophosphocholine; SAM = S-Adenosyl methionine

**Table S5: Diastolic dysfunction full results\***

Metabolite	Pathway	Sub-Pathway	Log Fold change	Unadjusted p-value	Adjusted p-value
azelate (nonanedioate; C9)	Lipid	Fatty Acid, Dicarboxylate	-0.33	0.001	0.49
1-arachidonoyl-GPE* (20:4)*	Lipid	Lysolipid	0.21	0.003	0.49
1-arachidonylglycerol	Lipid	Monoacylglycerol	0.25	0.004	0.49
2-arachidonoyl-GPC* (20:4)*	Lipid	Lysolipid	0.29	0.01	0.49
1-arachidonoyl-GPC* (20:4)*	Lipid	Lysolipid	0.24	0.01	0.49
palmitoyl-arachidonoyl-glycerophosphocholine (2)*	Lipid	Lysolipid	0.17	0.01	0.49
TL18:3n6 (g-linolenic acid)	Lipid	Mole % Total Fatty Acid	0.22	0.01	0.49
citrate	Energy	TCA Cycle	-0.17	0.01	0.49
1-docosahexaenoylglycerophosphoethanolamine*	Lipid	Lysolipid	0.26	0.01	0.49
2-palmitoleoyl-GPC* (16:1)*	Lipid	Lysolipid	0.48	0.01	0.49
N6-acetyllsine	Amino Acid	Lysine Metabolism	0.13	0.01	0.49
2-arachidonoyl-GPE* (20:4)*	Lipid	Lysolipid	0.47	0.01	0.49
xylitol	Carbohydrate	Pentose Metabolism	0.40	0.01	0.49
sulfate*	Xenobiotics	Chemical	0.09	0.01	0.59
myristoyl sphingomyelin*	Lipid	Sphingolipid Metabolism	0.12	0.01	0.59
1-palmitoyl-GPC (16:0)	Lipid	Lysolipid	0.19	0.01	0.59
cysteine s-sulfate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.18	0.02	0.59
S-methylcysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.23	0.02	0.59
ethylmalonate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.25	0.02	0.64
orotate	Nucleotide	Pyrimidine Metabolism, Orotate containing	0.37	0.02	0.64
orotidine	Nucleotide	Pyrimidine Metabolism, Orotate containing	0.50	0.02	0.65
2-myristoyl-GPC* (14:0)*	Lipid	Lysolipid	0.44	0.02	0.67
1-myristoyl-GPC (14:0)	Lipid	Lysolipid	0.31	0.02	0.67
TL20:3n9 (mead acid)	Lipid	Mole % Total Fatty Acid	0.30	0.03	0.67
1-stearoyl-GPE (18:0)	Lipid	Lysolipid	0.18	0.03	0.67
adrenate (22:4n6)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.18	0.03	0.67
1-linolenylglycerophosphocholine (18:3n3)*	Lipid	Lysolipid	0.27	0.03	0.67
arachidonate (20:4n6)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.12	0.03	0.67
biliverdin	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-0.41	0.03	0.67
2-hydroxy-3-methylvalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.20	0.03	0.67

<b>alpha-ketoglutarate</b>	Energy	TCA Cycle	0.22	0.04	0.67
<b>fucose</b>	Carbohydrate	Pentose Metabolism	0.21	0.04	0.67
<b>1-oleoyl-GPC (18:1)</b>	Lipid	Lysolipid	0.21	0.04	0.67
<b>2-stearoylglycerophosphoethanolamine*</b>	Lipid	Lysolipid	0.21	0.04	0.67
<b>3-methylglutaconate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.31	0.04	0.67
<b>1-palmitoleoyl-GPC* (16:1)*</b>	Lipid	Lysolipid	0.26	0.04	0.67
<b>2-palmitoyl-GPC* (16:0)*</b>	Lipid	Lysolipid	0.20	0.04	0.67
<b>hexadecanedioate (C16)</b>	Lipid	Fatty Acid, Dicarboxylate	-0.25	0.04	0.67
<b>1-stearoylglycerol (18:0)</b>	Lipid	Monoacylglycerol	0.59	0.04	0.67
<b>2'-deoxyuridine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.27	0.04	0.67
<b>2-docosahexaenoylglycerol*</b>	Lipid	Monoacylglycerol	0.66	0.04	0.68
<b>xanthosine</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.21	0.04	0.68
<b>1-eicosapentaenoylglycerophosphocholine (20:5n3)*</b>	Lipid	Lysolipid	0.36	0.05	0.68
<b>3-methylglutaryl carnitine (2)</b>	Amino Acid	Lysine Metabolism	0.31	0.05	0.68
<b>methyl glucopyranoside (alpha + beta)</b>	Xenobiotics	Food Component/Plant	-0.58	0.05	0.70
<b>N6-succinyladenosine</b>	Nucleotide	Purine Metabolism, Adenine containing	0.15	0.05	0.70
<b>sphinganine</b>	Lipid	Sphingolipid Metabolism	0.63	0.05	0.70
<b>1-stearoyl-GPC (18:0)</b>	Lipid	Lysolipid	0.22	0.05	0.70
<b>2-arachidonoyl glycerol</b>	Lipid	Monoacylglycerol	0.20	0.05	0.70
<b>5,6-dihydrothymine</b>	Nucleotide	Pyrimidine Metabolism, Thymine containing	-0.15	0.06	0.72
<b>phenylalanyl leucine</b>	Peptide	Dipeptide	0.57	0.06	0.72
<b>1-oleoyl-GPE (18:1)</b>	Lipid	Lysolipid	0.16	0.06	0.72
<b>3b-hydroxy-5-cholenoic acid</b>	Lipid	Secondary Bile Acid Metabolism	-0.47	0.06	0.72
<b>methionine sulfone</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.27	0.06	0.72
<b>stearoyl-arachidonoyl-glycerophosphoethanolamine (1)*</b>	Lipid	Lysolipid	0.20	0.06	0.72
<b>1-palmitoyl-GPE (16:0)</b>	Lipid	Lysolipid	0.16	0.06	0.72
<b>2-palmitoylglycerol (16:0)</b>	Lipid	Monoacylglycerol	0.29	0.06	0.72
<b>stearoyl-arachidonoyl-glycerophosphocholine (2)*</b>	Lipid	Lysolipid	0.13	0.07	0.72
<b>1-stearoylplasmylethanolamine*</b>	Lipid	Lysolipid	0.21	0.07	0.72
<b>1-docosapentaenoyl-GPC* (22:5n3)*</b>	Lipid	Lysolipid	0.20	0.07	0.72
<b>N-acetylputrescine</b>	Amino Acid	Polyamine Metabolism	0.18	0.07	0.72



<b>lanosterol</b>	Lipid	Sterol	-0.46	0.07	0.72
<b>1-pentadecanoylglycerophosphocholine (15:0)*</b>	Lipid	Lysolipid	0.18	0.07	0.72
<b>myristoylcarnitine</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.24	0.07	0.72
<b>1-docosahexaenoylglycerol</b>	Lipid	Monoacylglycerol	0.24	0.07	0.72
<b>tetradecanedioate (C14)</b>	Lipid	Fatty Acid, Dicarboxylate	-0.22	0.08	0.72
<b>eugenol sulfate</b>	Xenobiotics	Food Component/Plant	0.71	0.08	0.72
<b>2-oleoyl-GPC* (18:1)*</b>	Lipid	Lysolipid	0.17	0.08	0.72
<b>2-hydroxyisobutyrate</b>	Xenobiotics	Chemical	0.17	0.08	0.72
<b>propionylglycine (C3)</b>	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.21	0.08	0.72
<b>2-stearoyl-GPC* (18:0)*</b>	Lipid	Lysolipid	0.23	0.08	0.72
<b>1-linolenoylglycerol</b>	Lipid	Monoacylglycerol	0.20	0.08	0.74
<b>1-docosahexaenoyl-GPC* (22:6)*</b>	Lipid	Lysolipid	0.20	0.08	0.74
<b>1-palmitoylplasmenylethanolamine *</b>	Lipid	Lysolipid	0.13	0.08	0.74
<b>3-hydroxy-3-methylglutarate</b>	Lipid	Mevalonate Metabolism	0.12	0.09	0.74
<b>leucylalanine</b>	Peptide	Dipeptide	0.41	0.09	0.74
<b>caprylate (8:0)</b>	Lipid	Medium Chain Fatty Acid	-0.11	0.09	0.74
<b>indoleacetylglutamine</b>	Amino Acid	Tryptophan Metabolism	0.54	0.09	0.74
<b>palmitoyl-linoleoylglycerophosphocholine (2)*</b>	Lipid	Lysolipid	-0.11	0.09	0.74
<b>3-methoxytyrosine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.11	0.09	0.74
<b>malonate (propanedioate)</b>	Lipid	Fatty Acid Synthesis	-0.26	0.09	0.74
<b>ribitol</b>	Carbohydrate	Pentose Metabolism	0.10	0.09	0.74
<b>serylleucine</b>	Peptide	Dipeptide	-0.62	0.09	0.74
<b>benzoate</b>	Xenobiotics	Benzoate Metabolism	-0.11	0.10	0.79
<b>1,2,3-benzenetriol sulfate (2)</b>	Xenobiotics	Chemical	-0.74	0.10	0.79
<b>erythronate*</b>	Carbohydrate	Aminosugar Metabolism	0.10	0.11	0.82
<b>1-eicosatrienoyl-GPC* (20:3)*</b>	Lipid	Lysolipid	0.16	0.11	0.84
<b>2-eicosatrienoyl-GPC* (20:3)*</b>	Lipid	Lysolipid	0.14	0.11	0.84
<b>adenosine</b>	Nucleotide	Purine Metabolism, Adenine containing	-0.28	0.12	0.84
<b>3-methoxycatechol sulfate (1)</b>	Xenobiotics	Benzoate Metabolism	-0.57	0.12	0.84
<b>N-acetyltryptophan</b>	Amino Acid	Tryptophan Metabolism	0.17	0.12	0.84
<b>glycylvaline</b>	Peptide	Dipeptide	0.58	0.12	0.84
<b>phenyllactate (PLA)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.12	0.12	0.84
<b>glutamine</b>	Amino Acid	Glutamate Metabolism	-0.06	0.12	0.84
<b>dimethyl sulfone</b>	Xenobiotics	Chemical	0.48	0.12	0.84

<b>cytidine</b>	Nucleotide	Pyrimidine Metabolism, Cytidine containing	0.14	0.12	0.84
<b>alpha-hydroxyisovalerate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.18	0.13	0.85
<b>1-oleoylplasmenylethanolamine*</b>	Lipid	Lysolipid	0.15	0.13	0.86
<b>phenylalanylserine</b>	Peptide	Dipeptide	-0.50	0.13	0.87
<b>2-palmitoyl-GPE* (16:0)*</b>	Lipid	Lysolipid	0.17	0.14	0.87
<b>1-methyladenosine</b>	Nucleotide	Purine Metabolism, Adenine containing	0.08	0.14	0.87
<b>docosahexaenoate (DHA; 22:6n3)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.16	0.14	0.87
<b>3-methyl catechol sulfate (1)</b>	Xenobiotics	Benzoate Metabolism	0.45	0.14	0.87
<b>inositol 1-phosphate (I1P)</b>	Lipid	Inositol Metabolism	0.16	0.14	0.87
<b>caproate (6:0)</b>	Lipid	Medium Chain Fatty Acid	-0.09	0.14	0.87
<b>eicosenoyl sphingomyelin*</b>	Lipid	Sphingolipid Metabolism	0.12	0.14	0.87
<b>tyrosylglutamate</b>	Peptide	Dipeptide	0.38	0.14	0.87
<b>3-hydroxy-2-ethylpropionate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.11	0.14	0.87
<b>palmitoyl-linoleoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	-0.10	0.14	0.87
<b>stearoylcarnitine (C18)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.17	0.15	0.87
<b>2-docosahexaenoyl-GPC* (22:6)*</b>	Lipid	Lysolipid	0.21	0.16	0.89
<b>pyroglutamylglutamine</b>	Peptide	Dipeptide	0.24	0.16	0.89
<b>3-indoxyl sulfate</b>	Amino Acid	Tryptophan Metabolism	0.21	0.16	0.89
<b>eicosapentaenoate (EPA; 20:5n3)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.21	0.16	0.89
<b>cyclo(pro-pro)</b>	Peptide	Dipeptide	0.16	0.16	0.89
<b>methyl indole-3-acetate</b>	Xenobiotics	Food Component/Plant	0.20	0.16	0.89
<b>12-HETE</b>	Lipid	Eicosanoid	-0.36	0.16	0.89
<b>glutamate</b>	Amino Acid	Glutamate Metabolism	0.11	0.17	0.89
<b>aspartylphenylalanine</b>	Peptide	Dipeptide	0.31	0.17	0.89
<b>tyramine O-sulfate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.38	0.17	0.89
<b>2-arachidonoylglycerophosphoinositol*</b>	Lipid	Lysolipid	0.29	0.17	0.89
<b>3-methoxytyramine sulfate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.16	0.17	0.89
<b>cysteine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.14	0.18	0.89
<b>glycolithocholate sulfate*</b>	Lipid	Secondary Bile Acid Metabolism	-0.36	0.18	0.89
<b>mannose</b>	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.10	0.18	0.89
<b>3-ureidopropionate</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.13	0.18	0.89
<b>dodecanedioate (C12)</b>	Lipid	Fatty Acid, Dicarboxylate	-0.17	0.18	0.89

<b>N-methylproline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.33	0.18	0.89
<b>1,3-dimethylurate</b>	Xenobiotics	Xanthine Metabolism	-0.55	0.18	0.89
<b>1-arachidoyl-GPC (20:0)</b>	Lipid	Lysolipid	0.42	0.19	0.89
<b>1-eicosenoylglycerophosphocholine (20:1n9)*</b>	Lipid	Lysolipid	0.19	0.19	0.89
<b>phenylpyruvate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.10	0.19	0.89
<b>palmitoylcarnitine (C16)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.14	0.19	0.89
<b>docosapentaenoate (DPA; 22:5n3)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.13	0.19	0.89
<b>betaine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.08	0.19	0.89
<b>TL20:4n6 (arachidonic acid)</b>	Lipid	Mole % Total Fatty Acid	0.09	0.19	0.89
<b>kynurenate</b>	Amino Acid	Tryptophan Metabolism	-0.13	0.19	0.89
<b>oleoylcarnitine (C18)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.16	0.19	0.89
<b>octadecanedioate (C18)</b>	Lipid	Fatty Acid, Dicarboxylate	-0.16	0.20	0.89
<b>N2-methylguanosine</b>	Nucleotide	Purine Metabolism, Guanine containing	0.13	0.20	0.89
<b>TL20:2n6 (eicosadienoic acid)</b>	Lipid	Mole % Total Fatty Acid	0.10	0.20	0.89
<b>1-heptadecanoyl-GPC (17:0)</b>	Lipid	Lysolipid	0.23	0.20	0.89
<b>N6-methyladenosine</b>	Nucleotide	Purine Metabolism, Adenine containing	0.13	0.20	0.89
<b>5-HETE</b>	Lipid	Eicosanoid	0.22	0.20	0.89
<b>dimethylarginine (ADMA + SDMA)</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.04	0.20	0.89
<b>cis-Cyclo[L-ala-L-Pro]</b>	Peptide	Dipeptide	0.12	0.20	0.89
<b>N-acetylmethionine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.20	0.20	0.89
<b>gamma-glutamyllysine</b>	Peptide	Gamma-glutamyl Amino Acid	0.10	0.21	0.89
<b>stearate (18:0)</b>	Lipid	Long Chain Fatty Acid	0.06	0.21	0.89
<b>histidyltryptophan</b>	Peptide	Dipeptide	-0.26	0.21	0.89
<b>TL20:5n3 (eicosapentaenoic acid)</b>	Lipid	Mole % Total Fatty Acid	0.19	0.21	0.89
<b>imidazole propionate</b>	Amino Acid	Histidine Metabolism	0.24	0.21	0.89
<b>C-glycosyltryptophan</b>	Amino Acid	Tryptophan Metabolism	0.06	0.21	0.89
<b>phenylacetylglutamine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.21	0.21	0.89
<b>desmosterol</b>	Lipid	Sterol	-0.21	0.21	0.89
<b>glucuronate</b>	Carbohydrate	Aminosugar Metabolism	0.12	0.21	0.89
<b>cyclo(gly-pro)</b>	Peptide	Dipeptide	0.19	0.21	0.89
<b>sphingomyelin</b>	Lipid	Sphingolipid Metabolism	0.09	0.21	0.89
<b>4-hydroxyhippurate</b>	Xenobiotics	Benzoate Metabolism	-0.24	0.22	0.89
<b>TL18:2n6 (linoleic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.06	0.22	0.90

<b>16-hydroxypalmitate</b>	Lipid	Fatty Acid, Monohydroxy	-0.09	0.22	0.92
<b>allo-isoleucine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.08	0.23	0.92
<b>2-oleoyl-GPE* (18:1)*</b>	Lipid	Lysolipid	0.36	0.23	0.92
<b>docosapentaenoate (n6 DPA; 22:5n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.09	0.23	0.92
<b>9,10-DiHOME</b>	Lipid	Fatty Acid, Dihydroxy	-0.25	0.23	0.92
<b>TL22:5n3 (docosapentaenoic acid)</b>	Lipid	Mole % Total Fatty Acid	0.08	0.23	0.92
<b>2-aminooctanoate</b>	Lipid	Fatty Acid, Amino	0.15	0.24	0.92
<b>7-alpha-hydroxycholesterol</b>	Lipid	Sterol	0.21	0.24	0.92
<b>thyroxine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.32	0.24	0.92
<b>gamma-glutamylvaline</b>	Peptide	Gamma-glutamyl Amino Acid	0.06	0.24	0.92
<b>saccharin</b>	Xenobiotics	Food Component/Plant	0.70	0.24	0.92
<b>glucose</b>	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.06	0.24	0.92
<b>hypotaurine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.24	0.25	0.93
<b>10-undecenoate (11:1n1)</b>	Lipid	Medium Chain Fatty Acid	-0.11	0.25	0.93
<b>1-palmitoylglycerophosphate</b>	Lipid	Lysolipid	0.18	0.25	0.93
<b>salicylic glucuronide*</b>	Xenobiotics	Drug	0.60	0.25	0.93
<b>gamma-glutamylalanine</b>	Peptide	Gamma-glutamyl Amino Acid	0.11	0.25	0.93
<b>cholesterol</b>	Lipid	Sterol	-0.07	0.25	0.93
<b>taurothiocholate 3-sulfate</b>	Lipid	Secondary Bile Acid Metabolism	-0.38	0.25	0.93
<b>alanine</b>	Amino Acid	Alanine and Aspartate Metabolism	0.05	0.26	0.93
<b>taurocholate sulfate</b>	Lipid	Secondary Bile Acid Metabolism	-0.19	0.26	0.93
<b>stearidonate (18:4n3)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.14	0.26	0.93
<b>7-methylurate</b>	Xenobiotics	Xanthine Metabolism	-0.51	0.26	0.93
<b>serine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.07	0.26	0.93
<b>glutaryl carnitine (C5)</b>	Amino Acid	Lysine Metabolism	0.08	0.26	0.93
<b>1-dihomo-linolenylglycerol (alpha, gamma)</b>	Lipid	Monoacylglycerol	0.11	0.27	0.93
<b>lactate</b>	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.06	0.27	0.93
<b>pseudouridine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.05	0.27	0.93
<b>taurochenodeoxycholate</b>	Lipid	Primary Bile Acid Metabolism	-0.33	0.27	0.93
<b>N-acetyl-3-methylhistidine*</b>	Amino Acid	Histidine Metabolism	0.30	0.27	0.93
<b>oleoyl sphingomyelin</b>	Lipid	Sphingolipid Metabolism	0.07	0.28	0.93

<b>phenylacetate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.17	0.28	0.93
<b>delta-tocopherol</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.25	0.28	0.93
<b>1-arachidonoylglycerophosphate</b>	Lipid	Lysolipid	0.12	0.28	0.93
<b>4-acetamidobutanoate</b>	Amino Acid	Polyamine Metabolism	0.08	0.28	0.93
<b>theobromine</b>	Xenobiotics	Xanthine Metabolism	-0.33	0.28	0.93
<b>indolepropionate</b>	Amino Acid	Tryptophan Metabolism	-0.20	0.29	0.93
<b>butyrylcarnitine (C4)</b>	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.12	0.29	0.93
<b>salicylate</b>	Xenobiotics	Drug	0.43	0.29	0.93
<b>1,2-propanediol</b>	Xenobiotics	Chemical	0.23	0.29	0.93
<b>N-acetyl-1-methylhistidine*</b>	Amino Acid	Histidine Metabolism	0.15	0.29	0.93
<b>TL18:1n9 (oleic acid)</b>	Lipid	Mole % Total Fatty Acid	0.04	0.29	0.93
<b>1-eicosadienoyl-GPC* (20:2)*</b>	Lipid	Lysolipid	0.14	0.29	0.93
<b>N3-methyluridine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.14	0.29	0.93
<b>N-oleoyltaurine</b>	Lipid	Endocannabinoid	0.25	0.29	0.93
<b>N-acetylcarnosine</b>	Peptide	Dipeptide Derivative	-0.08	0.29	0.93
<b>pregnen-diol disulfate*</b>	Lipid	Steroid	0.16	0.30	0.93
<b>methionine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.05	0.30	0.93
<b>2-ethylhexanoic acid</b>	Xenobiotics	Chemical	-0.09	0.30	0.93
<b>gamma-CEHC glucuronide*</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.31	0.30	0.93
<b>caprate (10:0)</b>	Lipid	Medium Chain Fatty Acid	-0.10	0.30	0.93
<b>1-myristoylglycerol (14:0)</b>	Lipid	Monoacylglycerol	0.15	0.30	0.93
<b>gamma-glutamylisoleucine*</b>	Peptide	Gamma-glutamyl Amino Acid	0.07	0.31	0.93
<b>3-hydroxypyridine sulfate</b>	Xenobiotics	Chemical	0.29	0.31	0.93
<b>2-piperidinone</b>	Xenobiotics	Food Component/Plant	0.27	0.31	0.93
<b>2-linoleoyl-GPC* (18:2)*</b>	Lipid	Lysolipid	0.10	0.31	0.93
<b>12,13-DiHOME</b>	Lipid	Fatty Acid, Dihydroxy	-0.14	0.32	0.93
<b>4-methylcatechol sulfate</b>	Xenobiotics	Benzoate Metabolism	-0.24	0.32	0.93
<b>dopamine sulfate (2)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.11	0.32	0.93
<b>palmitoyl-arachidonoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	0.11	0.32	0.93
<b>N2-acetyllysine</b>	Amino Acid	Lysine Metabolism	0.15	0.32	0.93
<b>indolelactate</b>	Amino Acid	Tryptophan Metabolism	0.07	0.32	0.93
<b>arabonate</b>	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.09	0.32	0.93
<b>N-palmitoyl glycine</b>	Lipid	Fatty Acid Metabolism(Acyl Glycine)	-0.12	0.32	0.93
<b>6-oxopiperidine-2-carboxylic acid</b>	Xenobiotics	Drug	0.08	0.33	0.93
<b>arabitol</b>	Carbohydrate	Pentose Metabolism	0.08	0.33	0.93

<b>tryptophan betaine</b>	Amino Acid	Tryptophan Metabolism	0.25	0.33	0.93
<b>2-hydroxyhippurate (salicylurate)</b>	Xenobiotics	Benzoate Metabolism	0.39	0.33	0.93
<b>glycylphenylalanine</b>	Peptide	Dipeptide	-0.25	0.33	0.93
<b>5alpha-pregnan-3beta,20alpha-diol monosulfate (2)</b>	Lipid	Steroid	0.34	0.33	0.93
<b>myo-inositol</b>	Lipid	Inositol Metabolism	0.05	0.33	0.93
<b>2-stearoylglycerophosphoinositol*</b>	Lipid	Lysolipid	-0.16	0.34	0.93
<b>glycylproline</b>	Peptide	Dipeptide	-0.24	0.34	0.93
<b>5-methylthioadenosine (MTA)</b>	Amino Acid	Polyamine Metabolism	0.29	0.34	0.93
<b>adenosine 3',5'-cyclic monophosphate (cAMP)</b>	Nucleotide	Purine Metabolism, Adenine containing	0.21	0.34	0.93
<b>palmitoleoyl sphingomyelin*</b>	Lipid	Sphingolipid Metabolism	0.05	0.34	0.93
<b>5alpha-pregnan-3beta,20alpha-diol disulfate</b>	Lipid	Steroid	0.19	0.34	0.93
<b>erythritol</b>	Xenobiotics	Food Component/Plant	0.12	0.34	0.93
<b>methysuccinate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.07	0.34	0.93
<b>prolylhydroxyproline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.12	0.34	0.93
<b>gamma-glutamyl-2-aminobutyrate</b>	Peptide	Gamma-glutamyl Amino Acid	0.17	0.34	0.93
<b>p-cresol sulfate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.26	0.35	0.93
<b>TL22:6n3 (docosahexaenoic acid)</b>	Lipid	Mole % Total Fatty Acid	0.09	0.35	0.93
<b>hydroquinone sulfate</b>	Xenobiotics	Drug	-0.26	0.35	0.93
<b>2,3-dihydroxyisovalerate</b>	Xenobiotics	Food Component/Plant	0.32	0.35	0.93
<b>myristoleoylcarnitine*</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.14	0.35	0.93
<b>pantothenate (Vitamin B5)</b>	Cofactors and Vitamins	Pantothenate and CoA Metabolism	0.11	0.35	0.93
<b>dihomolinolenate (20:3n3 or 3n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.05	0.35	0.93
<b>dihomolinoleate (20:2n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.09	0.35	0.93
<b>5,6-dihydrouracil</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.07	0.36	0.93
<b>1-linoleoyl-GPC (18:2)</b>	Lipid	Lysolipid	0.07	0.36	0.93
<b>paraxanthine</b>	Xenobiotics	Xanthine Metabolism	-0.44	0.36	0.93
<b>3-hydroxymyristate</b>	Lipid	Fatty Acid, Monohydroxy	0.08	0.36	0.93
<b>valylarginine</b>	Peptide	Dipeptide	0.23	0.36	0.93
<b>coprostanol</b>	Lipid	Sterol	0.28	0.36	0.93
<b>imidazole lactate</b>	Amino Acid	Histidine Metabolism	0.08	0.36	0.93
<b>pregnenolone sulfate</b>	Lipid	Steroid	0.19	0.36	0.93
<b>TL15:0 (pentadecanoic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.04	0.37	0.93
<b>alpha-hydroxyisocaproate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.08	0.37	0.93

<b>docosadienoate (22:2n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.08	0.37	0.93
<b>N-acetylneuramate</b>	Carbohydrate	Aminosugar Metabolism	0.10	0.37	0.93
<b>N-acetyltaurine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.11	0.38	0.93
<b>laurylcarnitine (C12)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.10	0.38	0.93
<b>7-dehydro-cholesterol</b>	Lipid	Sterol	0.31	0.38	0.93
<b>2-aminobutyrate</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.07	0.38	0.93
<b>1-palmitoylglycerol (16:0)</b>	Lipid	Monoacylglycerol	0.08	0.38	0.93
<b>N-acetylaspartate (NAA)</b>	Amino Acid	Alanine and Aspartate Metabolism	-0.05	0.38	0.93
<b>1-linoleoylglycerol (18:2)</b>	Lipid	Monoacylglycerol	0.09	0.38	0.93
<b>N-acetyl-aspartyl-glutamate (NAAG)</b>	Amino Acid	Glutamate Metabolism	-0.06	0.38	0.93
<b>5-oxoproline</b>	Amino Acid	Glutathione Metabolism	-0.07	0.39	0.93
<b>glycochenodeoxycholate</b>	Lipid	Primary Bile Acid Metabolism	-0.21	0.39	0.93
<b>glycocholenate sulfate*</b>	Lipid	Secondary Bile Acid Metabolism	-0.09	0.39	0.93
<b>hippurate</b>	Xenobiotics	Benzoate Metabolism	-0.18	0.39	0.94
<b>1-methylnicotinamide</b>	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-0.23	0.39	0.94
<b>N-6-trimethyllysine</b>	Amino Acid	Lysine Metabolism	-0.09	0.39	0.94
<b>10-nonadecenoate (19:1n9)</b>	Lipid	Long Chain Fatty Acid	0.08	0.40	0.94
<b>dihydroorotate</b>	Nucleotide	Pyrimidine Metabolism, Orotate containing	0.20	0.40	0.94
<b>tyrosine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.04	0.40	0.94
<b>21-hydroxypregnenolone disulfate</b>	Lipid	Steroid	0.14	0.40	0.94
<b>glycoursodeoxycholate</b>	Lipid	Secondary Bile Acid Metabolism	-0.29	0.40	0.94
<b>4-hydroxychlorothalonil</b>	Xenobiotics	Chemical	0.11	0.41	0.95
<b>oxalate (ethanedioate)</b>	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	-0.13	0.41	0.95
<b>catechol sulfate</b>	Xenobiotics	Benzoate Metabolism	-0.17	0.41	0.95
<b>glycolate (hydroxyacetate)</b>	Xenobiotics	Chemical	-0.05	0.41	0.95
<b>2-methylmalonyl carnitine</b>	Lipid	Fatty Acid Synthesis	-0.07	0.42	0.95
<b>isovalerylcarnitine (C5)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.08	0.42	0.95
<b>stigmasterol</b>	Lipid	Sterol	-0.15	0.42	0.95
<b>dopamine sulfate (1)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.13	0.42	0.95
<b>alpha-glutamyltyrosine</b>	Peptide	Dipeptide	-0.26	0.42	0.95
<b>arachidate (20:0)</b>	Lipid	Long Chain Fatty Acid	0.05	0.43	0.95
<b>beta-hydroxyisovalerate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.08	0.43	0.95
<b>palmitoyl sphingomyelin</b>	Lipid	Sphingolipid Metabolism	0.03	0.43	0.95

<b>asparagine</b>	Amino Acid	Alanine and Aspartate Metabolism	-0.03	0.43	0.95
<b>piperine</b>	Xenobiotics	Food Component/Plant	0.17	0.43	0.95
<b>oleoyl-linoleoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	0.04	0.43	0.95
<b>cholestanol</b>	Lipid	Sterol	-0.07	0.43	0.95
<b>alpha-tocopherol</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.08	0.43	0.95
<b>cyclohexanebutanoic acid</b>	Xenobiotics	Chemical	-0.09	0.43	0.95
<b>inosine</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.23	0.43	0.95
<b>eicosanodioate</b>	Lipid	Fatty Acid, Dicarboxylate	-0.10	0.44	0.95
<b>3beta,7alpha-dihydroxy-5-cholestenoate</b>	Lipid	Secondary Bile Acid Metabolism	0.24	0.44	0.95
<b>xanthine</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.08	0.44	0.95
<b>eicosenoate (20:1n9 or 1n11)</b>	Lipid	Long Chain Fatty Acid	0.07	0.44	0.95
<b>isobutyrylglycine (C4)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.09	0.44	0.95
<b>2-hydroxyoctanoate</b>	Lipid	Fatty Acid, Monohydroxy	0.08	0.44	0.95
<b>proline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.04	0.44	0.95
<b>ribonate (ribonolactone)</b>	Carbohydrate	Pentose Metabolism	-0.07	0.45	0.95
<b>3-methyl-2-oxobutyrate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.04	0.45	0.95
<b>ectoine</b>	Xenobiotics	Chemical	0.20	0.45	0.95
<b>linoleoylcarnitine*</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.10	0.45	0.95
<b>pyruvate</b>	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.11	0.46	0.95
<b>hydantoin-5-propionic acid</b>	Amino Acid	Histidine Metabolism	0.17	0.46	0.95
<b>cysteine-glutathione disulfide</b>	Amino Acid	Glutathione Metabolism	-0.20	0.46	0.95
<b>3-hydroxybutyrate (BHBA)</b>	Lipid	Ketone Bodies	-0.14	0.46	0.95
<b>histidylphenylalanine</b>	Peptide	Dipeptide	0.21	0.47	0.95
<b>allantoin</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.11	0.47	0.95
<b>1,3,7-trimethylurate</b>	Xenobiotics	Xanthine Metabolism	-0.24	0.47	0.95
<b>mannitol</b>	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.22	0.47	0.95
<b>alpha-ketobutyrate</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.14	0.47	0.95
<b>squalene</b>	Lipid	Sterol	0.20	0.47	0.95
<b>3-(4-hydroxyphenyl)propionate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.27	0.47	0.95
<b>pyridoxine (Vitamin B6)</b>	Cofactors and Vitamins	Vitamin B6 Metabolism	-0.06	0.47	0.95



<b>TL16:1n7 (palmitoleic acid)</b>	Lipid	Mole % Total Fatty Acid	0.07	0.47	0.95
<b>ornithine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.06	0.47	0.95
<b>pelargonate (9:0)</b>	Lipid	Medium Chain Fatty Acid	-0.04	0.47	0.95
<b>beta-tocopherol</b>	Cofactors and Vitamins	Tocopherol Metabolism	-0.15	0.48	0.95
<b>taurine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.07	0.48	0.95
<b>aspartate</b>	Amino Acid	Alanine and Aspartate Metabolism	0.07	0.48	0.95
<b>TL20:1n9 (eicosaenoic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.03	0.48	0.95
<b>1-methylhistidine</b>	Amino Acid	Histidine Metabolism	0.07	0.48	0.95
<b>taurocholate</b>	Lipid	Primary Bile Acid Metabolism	-0.25	0.48	0.95
<b>5alpha-androstan-3beta,17beta-diol disulfate</b>	Lipid	Steroid	-0.18	0.48	0.95
<b>N-formylmethionine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.03	0.49	0.95
<b>4-androsten-3beta,17beta-diol disulfate (1)</b>	Lipid	Steroid	0.15	0.49	0.95
<b>tryptophylglutamate</b>	Peptide	Dipeptide	-0.27	0.49	0.95
<b>4-allylphenol sulfate</b>	Xenobiotics	Food Component/Plant	0.17	0.49	0.96
<b>chenodeoxycholate</b>	Lipid	Primary Bile Acid Metabolism	-0.17	0.49	0.96
<b>arginine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.05	0.50	0.96
<b>palmitate (16:0)</b>	Lipid	Long Chain Fatty Acid	0.03	0.50	0.96
<b>ADSGEGDFAEGGGVR*</b>	Peptide	Fibrinogen Cleavage Peptide	-0.06	0.50	0.96
<b>phenol sulfate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.18	0.50	0.96
<b>1,5-anhydroglucitol (1,5-AG)</b>	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	-0.09	0.50	0.97
<b>O-sulfo-L-tyrosine</b>	Xenobiotics	Chemical	0.05	0.51	0.97
<b>valine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.03	0.51	0.97
<b>gamma-glutamylleucine</b>	Peptide	Gamma-glutamyl Amino Acid	0.04	0.51	0.97
<b>N-acetylphenylalanine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.07	0.51	0.97
<b>seryltyrosine</b>	Peptide	Dipeptide	0.15	0.51	0.97
<b>serylalanine</b>	Peptide	Dipeptide	0.10	0.51	0.97
<b>glycylglycine</b>	Peptide	Dipeptide	-0.28	0.52	0.97
<b>N-acetylglutamate</b>	Amino Acid	Glutamate Metabolism	0.16	0.52	0.97
<b>5alpha-pregnan-3beta,20beta-diol monosulfate (1)</b>	Lipid	Steroid	-0.15	0.52	0.97
<b>TLdm18:1n9 (plasmalogen oleic acid)</b>	Lipid	Mole % Total Fatty Acid	0.06	0.52	0.97
<b>indolebutyrate</b>	Amino Acid	Tryptophan Metabolism	0.13	0.52	0.97
<b>3-hydroxyoctanoate</b>	Lipid	Fatty Acid, Monohydroxy	-0.07	0.52	0.97

<b>4-hydroxyphenylpyruvate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.08	0.53	0.97
<b>5-hydroxyindoleacetate</b>	Amino Acid	Tryptophan Metabolism	0.06	0.53	0.97
<b>urea</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.05	0.53	0.97
<b>homovanillate (HVA)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.07	0.53	0.97
<b>3-methylhistidine</b>	Amino Acid	Histidine Metabolism	0.15	0.53	0.97
<b>threonate</b>	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	-0.10	0.53	0.97
<b>N-acetyl glycine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	0.08	0.53	0.97
<b>citrulline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.06	0.54	0.97
<b>fructose</b>	Carbohydrate	Fructose, Mannose and Galactose Metabolism	-0.05	0.54	0.97
<b>caffeine</b>	Xenobiotics	Xanthine Metabolism	-0.27	0.54	0.97
<b>theophylline</b>	Xenobiotics	Xanthine Metabolism	-0.24	0.54	0.97
<b>beta-hydroxyisovalerylcarnitine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.05	0.54	0.97
<b>hexanoylcarnitine (C6)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.05	0.54	0.97
<b>1-arachidonoyl-GPI* (20:4)*</b>	Lipid	Lysolipid	0.04	0.54	0.97
<b>indoleacetate</b>	Amino Acid	Tryptophan Metabolism	0.07	0.55	0.97
<b>2-aminoheptanoate</b>	Lipid	Fatty Acid, Amino	0.06	0.55	0.97
<b>sorbitol</b>	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.10	0.55	0.97
<b>4-androsten-3beta,17beta-diol monosulfate (1)</b>	Lipid	Steroid	0.12	0.55	0.97
<b>N-acetylalanine</b>	Amino Acid	Alanine and Aspartate Metabolism	0.02	0.55	0.97
<b>palmitoyl-oleoyl-glycerophosphoglycerol (2)*</b>	Lipid	Lysolipid	0.19	0.56	0.97
<b>N-acetyltyrosine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.06	0.56	0.97
<b>1-eicosatrienoylglycerophosphoethanolamine*</b>	Lipid	Lysolipid	0.14	0.56	0.97
<b>adenine</b>	Nucleotide	Purine Metabolism, Adenine containing	0.07	0.56	0.98
<b>3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)</b>	Lipid	Fatty Acid, Dicarboxylate	0.21	0.56	0.98
<b>glycine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.04	0.57	0.98
<b>1,7-dimethylurate</b>	Xenobiotics	Xanthine Metabolism	-0.22	0.57	0.98
<b>galactonate</b>	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.25	0.57	0.98
<b>homostachydrine*</b>	Xenobiotics	Food Component/Plant	0.07	0.57	0.98
<b>1-methylxanthine</b>	Xenobiotics	Xanthine Metabolism	0.18	0.57	0.98
<b>methionine sulfoxide</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.05	0.57	0.98
<b>2-hydroxydecanoate</b>	Lipid	Fatty Acid, Monohydroxy	0.07	0.58	0.98

<b>quinolinate</b>	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.09	0.58	0.98
<b>isoleucine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.02	0.58	0.98
<b>3-hydroxyisobutyrate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.05	0.58	0.98
<b>threonine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.03	0.59	0.98
<b>malate</b>	Energy	TCA Cycle	-0.04	0.59	0.98
<b>isoleucylglycine</b>	Peptide	Dipeptide	-0.12	0.59	0.98
<b>N-(2-furoyl)glycine</b>	Xenobiotics	Food Component/Plant	0.10	0.59	0.98
<b>lathosterol</b>	Lipid	Sterol	-0.09	0.59	0.98
<b>phenylalanine</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.02	0.59	0.98
<b>andro steroid monosulfate (1)*</b>	Lipid	Steroid	0.14	0.59	0.98
<b>stearoyl-arachidonoyl-glycerophosphoinositol (1)*</b>	Lipid	Lysolipid	0.04	0.59	0.98
<b>1-oleoyl-GPI (18:1)*</b>	Lipid	Lysolipid	0.07	0.59	0.98
<b>stearoyl-linoleoyl-glycerophosphoethanolamine (1)*</b>	Lipid	Lysolipid	-0.07	0.60	0.99
<b>gamma-glutamyltryptophan</b>	Peptide	Gamma-glutamyl Amino Acid	0.04	0.60	0.99
<b>1-oleoylglycerol (18:1)</b>	Lipid	Monoacylglycerol	0.06	0.61	0.99
<b>13-HODE + 9-HODE</b>	Lipid	Fatty Acid, Monohydroxy	-0.07	0.61	0.99
<b>guanosine</b>	Nucleotide	Purine Metabolism, Guanine containing	-0.17	0.61	0.99
<b>3-(4-hydroxyphenyl)lactate (HPLA)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.03	0.61	0.99
<b>3-hydroxylaurate</b>	Lipid	Fatty Acid, Monohydroxy	0.05	0.61	0.99
<b>phenylalanyltryptophan</b>	Peptide	Dipeptide	0.08	0.62	0.99
<b>TL22:1n9 (erucic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.10	0.62	0.99
<b>5-methyluridine (ribothymidine)</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.03	0.62	0.99
<b>4-androsten-3beta,17beta-diol disulfate (2)</b>	Lipid	Steroid	0.07	0.63	0.99
<b>acisoga</b>	Amino Acid	Polyamine Metabolism	0.04	0.63	0.99
<b>TL14:0 (myristic acid)</b>	Lipid	Mole % Total Fatty Acid	0.05	0.63	0.99
<b>gamma-tocopherol</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.07	0.63	0.99
<b>4-guanidinobutanoate</b>	Amino Acid	Guanidino and Acetamido Metabolism	0.15	0.63	0.99
<b>3-phenylpropionate (hydrocinnamate)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.13	0.63	0.99
<b>N-acetylserine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	0.02	0.63	0.99
<b>pregn steroid monosulfate*</b>	Lipid	Steroid	0.07	0.64	0.99
<b>TLdm18:1n7 (plasmalogen vaccenic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.10	0.64	0.99
<b>isovalerylglycine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.06	0.64	0.99

<b>O-methylcatechol sulfate</b>	Xenobiotics	Benzoate Metabolism	-0.10	0.64	0.99
<b>TL22:5n6 (osbond acid)</b>	Lipid	Mole % Total Fatty Acid	0.04	0.64	0.99
<b>serotonin (5HT)</b>	Amino Acid	Tryptophan Metabolism	0.12	0.64	0.99
<b>beta-alanine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.05	0.64	0.99
<b>homocitrulline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.06	0.65	0.99
<b>quinat</b>	Xenobiotics	Food Component/Plant	0.22	0.65	0.99
<b>dimethylglycine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	0.04	0.65	0.99
<b>gamma-CEHC</b>	Cofactors and Vitamins	Tocopherol Metabolism	0.06	0.65	0.99
<b>creatine</b>	Amino Acid	Creatine Metabolism	0.05	0.65	0.99
<b>palmitoyl ethanolamide</b>	Lipid	Endocannabinoid	0.03	0.65	0.99
<b>gentisate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.19	0.65	0.99
<b>7-methylguanine</b>	Nucleotide	Purine Metabolism, Guanine containing	-0.02	0.65	0.99
<b>stearoyl-linoleoyl-glycerophosphocholine (2)*</b>	Lipid	Lysolipid	-0.03	0.66	0.99
<b>2-linoleoyl-GPE* (18:2)*</b>	Lipid	Lysolipid	0.05	0.66	0.99
<b>N2,N5-diacetylornithine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.09	0.66	0.99
<b>cholate</b>	Lipid	Primary Bile Acid Metabolism	-0.17	0.66	0.99
<b>N-acetylvaline</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.02	0.66	0.99
<b>octanoylcarnitine (C8)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.04	0.66	0.99
<b>isobutyrylcarnitine (C4)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.05	0.66	0.99
<b>lysine</b>	Amino Acid	Lysine Metabolism	0.02	0.66	0.99
<b>trans-urocanate</b>	Amino Acid	Histidine Metabolism	-0.05	0.67	0.99
<b>tiglyl carnitine (C5)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.04	0.67	0.99
<b>phenylcarnitine*</b>	Xenobiotics	Chemical	-0.13	0.67	0.99
<b>uridine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.02	0.68	0.99
<b>4-androsten-3alpha,17alpha-diol monosulfate (2)</b>	Lipid	Steroid	0.10	0.68	0.99
<b>gamma-glutamylphenylalanine</b>	Peptide	Gamma-glutamyl Amino Acid	0.02	0.68	0.99
<b>stearoyl-arachidonoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	-0.08	0.68	0.99
<b>xylose</b>	Carbohydrate	Pentose Metabolism	0.08	0.69	0.99
<b>gamma-glutamylglutamate</b>	Peptide	Gamma-glutamyl Amino Acid	0.06	0.69	0.99
<b>TL18:1n7 (avaccenic acid)</b>	Lipid	Mole % Total Fatty Acid	0.02	0.69	0.99
<b>myristate (14:0)</b>	Lipid	Long Chain Fatty Acid	0.03	0.69	0.99
<b>tartronate (hydroxymalonate)</b>	Xenobiotics	Bacterial/Fungal	-0.06	0.69	0.99

<b>1-methylimidazoleacetate</b>	Amino Acid	Histidine Metabolism	0.07	0.70	0.99
<b>bilirubin (E,E)*</b>	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	0.07	0.70	0.99
<b>prolylglycine</b>	Peptide	Dipeptide	-0.07	0.70	0.99
<b>glycocholate</b>	Lipid	Primary Bile Acid Metabolism	-0.10	0.70	0.99
<b>gamma-glutamylthreonine*</b>	Peptide	Gamma-glutamyl Amino Acid	0.03	0.70	0.99
<b>gamma-glutamylglutamine</b>	Peptide	Gamma-glutamyl Amino Acid	-0.03	0.70	0.99
<b>N-acetylleucine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.03	0.70	0.99
<b>TL22:4n6 (adrenic acid)</b>	Lipid	Mole % Total Fatty Acid	0.03	0.70	0.99
<b>arabinose</b>	Carbohydrate	Pentose Metabolism	0.08	0.70	0.99
<b>S-adenosylhomocysteine (SAH)</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.05	0.71	0.99
<b>androsterone sulfate</b>	Lipid	Steroid	-0.09	0.71	0.99
<b>docosatrienoate (22:3n3)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.04	0.71	0.99
<b>nicotinamide</b>	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-0.05	0.71	0.99
<b>trimethylamine N-oxide</b>	Lipid	Phospholipid Metabolism	0.16	0.71	0.99
<b>dehydroisoandrosterone sulfate (DHEA-S)</b>	Lipid	Steroid	0.07	0.72	0.99
<b>1,6-anhydroglucose</b>	Xenobiotics	Food Component/Plant	-0.08	0.72	0.99
<b>acetoacetate</b>	Lipid	Ketone Bodies	-0.05	0.72	0.99
<b>alpha-hydroxycaproate</b>	Lipid	Fatty Acid, Monohydroxy	0.03	0.72	0.99
<b>oleic ethanolamide</b>	Lipid	Endocannabinoid	0.03	0.72	0.99
<b>DSGEGDFXAEGGGVR*</b>	Peptide	Fibrinogen Cleavage Peptide	-0.09	0.72	0.99
<b>4-methyl-2-oxopentanoate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.02	0.72	0.99
<b>pregnanediol-3-glucuronide</b>	Lipid	Steroid	0.11	0.73	0.99
<b>3beta,7beta-dihydroxy-5-cholestenoate</b>	Lipid	Sterol	-0.03	0.73	0.99
<b>1-methylguanosine</b>	Nucleotide	Purine Metabolism, Guanine containing	-0.02	0.73	0.99
<b>N-acetylcitrulline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.09	0.73	0.99
<b>1-palmitoleoyl-GPI* (16:1)*</b>	Lipid	Lysolipid	0.14	0.73	0.99
<b>valerylcarnitine (C5)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.13	0.74	0.99
<b>10-heptadecenoate (17:1n7)</b>	Lipid	Long Chain Fatty Acid	0.04	0.74	0.99
<b>4-vinylphenol sulfate</b>	Xenobiotics	Benzoate Metabolism	0.10	0.74	0.99
<b>2-methylbutyrylcarnitine (C5)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.03	0.74	0.99
<b>TL14:1n5 (myristoleic acid)</b>	Lipid	Mole % Total Fatty Acid	0.05	0.74	0.99
<b>3,7-dimethylurate</b>	Xenobiotics	Xanthine Metabolism	-0.10	0.74	0.99
<b>nonadecanoate (19:0)</b>	Lipid	Long Chain Fatty Acid	0.02	0.74	0.99

<b>cyclo(leu-pro)</b>	Peptide	Dipeptide	0.06	0.75	0.99
<b>hexanoylglycine (C6)</b>	Lipid	Fatty Acid Metabolism(Acyl Glycine)	0.10	0.75	0.99
<b>3-methylglutaryl carnitine (1)</b>	Amino Acid	Lysine Metabolism	0.05	0.75	0.99
<b>stachydrine</b>	Xenobiotics	Food Component/Plant	0.09	0.75	0.99
<b>cortisol</b>	Lipid	Steroid	-0.04	0.75	0.99
<b>N-acetylarginine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.04	0.75	0.99
<b>tryptophan</b>	Amino Acid	Tryptophan Metabolism	-0.01	0.76	0.99
<b>2-hydroxystearate</b>	Lipid	Fatty Acid, Monohydroxy	0.02	0.76	0.99
<b>N-acetylisoleucine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.04	0.76	0.99
<b>N2,N2-dimethylguanosine</b>	Nucleotide	Purine Metabolism, Guanine containing	0.02	0.76	0.99
<b>gamma-glutamylmethionine</b>	Peptide	Gamma-glutamyl Amino Acid	0.03	0.77	0.99
<b>methylpalmitate (15 or 2)</b>	Lipid	Fatty Acid, Branched	0.02	0.77	0.99
<b>succinate</b>	Energy	TCA Cycle	0.01	0.77	0.99
<b>4-ureidobutyrate</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.04	0.77	0.99
<b>phenylalanylphenylalanine</b>	Peptide	Dipeptide	-0.04	0.77	0.99
<b>levulinate (4-oxovalerate)</b>	Xenobiotics	Food Component/Plant	0.03	0.77	0.99
<b>leucine</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.01	0.77	0.99
<b>3-hydroxyhippurate</b>	Xenobiotics	Benzoate Metabolism	-0.10	0.78	0.99
<b>2-linolenoylglycerophosphocholine(18:3n3)*</b>	Lipid	Lysolipid	-0.09	0.78	0.99
<b>cis-4-decenoyl carnitine</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.03	0.78	0.99
<b>homoarginine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.08	0.78	0.99
<b>1-pentadecanoylglycerol (1-monopentadecanoin)</b>	Lipid	Monoacylglycerol	-0.03	0.78	0.99
<b>pyridoxal</b>	Cofactors and Vitamins	Vitamin B6 Metabolism	-0.10	0.79	0.99
<b>maleate (cis-Butenedioate)</b>	Lipid	Fatty Acid, Dicarboxylate	0.04	0.79	0.99
<b>p-cresol-glucuronide*</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.12	0.79	0.99
<b>urate</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.02	0.79	0.99
<b>N-acetylglutamine</b>	Amino Acid	Glutamate Metabolism	0.03	0.79	0.99
<b>4-ethylphenyl sulfate</b>	Xenobiotics	Benzoate Metabolism	0.06	0.80	0.99
<b>isovalerate (C5)</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.02	0.80	0.99
<b>pentadecanoate (15:0)</b>	Lipid	Long Chain Fatty Acid	-0.02	0.80	0.99
<b>TL20:0 (arachidic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.02	0.80	0.99
<b>etiocholanolone glucuronide</b>	Lipid	Steroid	-0.07	0.80	0.99

<b>thymol sulfate</b>	Xenobiotics	Food Component/Plant	-0.11	0.80	0.99
<b>TL24:0 (lignoceric acid)</b>	Lipid	Mole % Total Fatty Acid	0.03	0.80	0.99
<b>campesterol</b>	Lipid	Sterol	-0.03	0.80	0.99
<b>5alpha-pregnan-3(alpha or beta),20beta-diol disulfate</b>	Lipid	Steroid	0.12	0.80	0.99
<b>o-cresol sulfate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.14	0.80	0.99
<b>2-linoleoylglycerol (2-monolinolein)</b>	Lipid	Monoacylglycerol	-0.04	0.81	0.99
<b>tyrosylglutamine</b>	Peptide	Dipeptide	-0.04	0.81	0.99
<b>succinylcarnitine (C4)</b>	Energy	TCA Cycle	-0.02	0.81	0.99
<b>N-acetyl-beta-alanine</b>	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.02	0.81	0.99
<b>1-methylurate</b>	Xenobiotics	Xanthine Metabolism	-0.06	0.81	0.99
<b>glycerol 3-phosphate (G3P)</b>	Lipid	Glycerolipid Metabolism	-0.05	0.82	0.99
<b>7-methylxanthine</b>	Xenobiotics	Xanthine Metabolism	-0.07	0.82	0.99
<b>7-HOCA</b>	Lipid	Sterol	-0.02	0.82	0.99
<b>trigonelline (N'-methylnicotinate)</b>	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-0.05	0.82	0.99
<b>TL24:1n9 (nervonic acid)</b>	Lipid	Mole % Total Fatty Acid	0.02	0.82	0.99
<b>guanidinoacetate</b>	Amino Acid	Creatine Metabolism	0.02	0.82	0.99
<b>5-acetylamino-6-amino-3-methyluracil</b>	Xenobiotics	Xanthine Metabolism	0.09	0.83	0.99
<b>maltose</b>	Carbohydrate	Glycogen Metabolism	0.05	0.83	0.99
<b>glucarate 1,4-lactone</b>	Carbohydrate	Disaccharides and Oligosaccharides	0.15	0.83	0.99
<b>margarate (17:0)</b>	Lipid	Long Chain Fatty Acid	0.02	0.83	0.99
<b>TL18:3n3 (a-linolenic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.02	0.83	0.99
<b>propionylcarnitine (C3)</b>	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	-0.02	0.83	0.99
<b>acetylcarnitine (C2)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.02	0.83	0.99
<b>threonylphenylalanine</b>	Peptide	Dipeptide	-0.08	0.83	0.99
<b>1-docosapentaenoyl-GPC* (22:5n6)*</b>	Lipid	Lysolipid	0.06	0.83	0.99
<b>ursodeoxycholate</b>	Lipid	Secondary Bile Acid Metabolism	-0.08	0.84	0.99
<b>2-hydroxybutyrate (AHB)</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.02	0.84	0.99
<b>palmitoleate (16:1n7)</b>	Lipid	Long Chain Fatty Acid	0.02	0.84	0.99
<b>creatinine</b>	Amino Acid	Creatine Metabolism	0.01	0.85	0.99
<b>TL20:4n3 (eicosatetraoic acid)</b>	Lipid	Mole % Total Fatty Acid	0.02	0.85	0.99
<b>threitol</b>	Carbohydrate	Pentose Metabolism	-0.02	0.85	0.99
<b>2-oleoylglycerol (18:1)</b>	Lipid	Monoacylglycerol	0.02	0.85	0.99
<b>indole-3-carboxylic acid</b>	Amino Acid	Tryptophan Metabolism	-0.01	0.85	0.99
<b>TLdm16:0 (plasmalogen palmitic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.01	0.86	0.99

<b>histidine</b>	Amino Acid	Histidine Metabolism	-0.02	0.86	0.99
<b>glycerol</b>	Lipid	Glycerolipid Metabolism	0.01	0.86	0.99
<b>pyroglutamine*</b>	Amino Acid	Glutamate Metabolism	-0.03	0.86	0.99
<b>N-acetylthreonine</b>	Amino Acid	Glycine, Serine and Threonine Metabolism	0.02	0.86	0.99
<b>pyroglutamylglycine</b>	Peptide	Dipeptide	-0.04	0.87	0.99
<b>N6-carbamoylthreonyladenosine</b>	Nucleotide	Purine Metabolism, Adenine containing	0.01	0.87	0.99
<b>myristoleoyl sphingomyelin*</b>	Lipid	Sphingolipid Metabolism	0.02	0.87	0.99
<b>5-dodecenoate (12:1n7)</b>	Lipid	Medium Chain Fatty Acid	-0.02	0.87	0.99
<b>5alpha-androstan-3beta,17alpha-diol disulfate</b>	Lipid	Steroid	0.05	0.87	0.99
<b>ribose</b>	Carbohydrate	Pentose Metabolism	0.03	0.87	0.99
<b>5alpha-androstan-3alpha,17beta-diol monosulfate (1)</b>	Lipid	Steroid	0.06	0.87	0.99
<b>gamma-glutamylhistidine</b>	Peptide	Gamma-glutamyl Amino Acid	-0.04	0.87	0.99
<b>N-delta-acetylornithine</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.02	0.87	0.99
<b>vaccenate (18:1n7)</b>	Lipid	Long Chain Fatty Acid	0.01	0.87	0.99
<b>decanoylcarnitine (C10)</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.01	0.87	0.99
<b>N-acetylhistidine</b>	Amino Acid	Histidine Metabolism	0.03	0.88	0.99
<b>17-methylstearate</b>	Lipid	Fatty Acid, Branched	0.02	0.88	0.99
<b>16a-hydroxy DHEA 3-sulfate</b>	Lipid	Steroid	0.03	0.88	0.99
<b>erucate (22:1n9)</b>	Lipid	Long Chain Fatty Acid	0.01	0.88	0.99
<b>xylonate</b>	Carbohydrate	Pentose Metabolism	0.03	0.88	0.99
<b>1-linoleoyl-GPI* (18:2)*</b>	Lipid	Lysolipid	0.01	0.88	0.99
<b>palmitoyl-linoleoyl-glycerophosphoinositol (1)*</b>	Lipid	Lysolipid	-0.03	0.88	0.99
<b>phosphate</b>	Energy	Oxidative Phosphorylation	-0.01	0.88	0.99
<b>cyclo(L-phe-L-pro)</b>	Peptide	Dipeptide	0.03	0.89	0.99
<b>myristoleate (14:1n5)</b>	Lipid	Long Chain Fatty Acid	-0.04	0.89	0.99
<b>glycerophosphoethanolamine</b>	Lipid	Phospholipid Metabolism	0.02	0.89	0.99
<b>kynurenine</b>	Amino Acid	Tryptophan Metabolism	0.01	0.89	0.99
<b>tartarate</b>	Xenobiotics	Food Component/Plant	0.04	0.89	0.99
<b>beta-sitosterol</b>	Lipid	Sterol	-0.02	0.90	0.99
<b>linoleate (18:2n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.01	0.90	0.99
<b>glycolithocholate</b>	Lipid	Secondary Bile Acid Metabolism	-0.05	0.90	0.99
<b>glycerate</b>	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.01	0.91	0.99
<b>glutarate (pentanedioate)</b>	Amino Acid	Lysine Metabolism	0.02	0.91	0.99
<b>fumarate</b>	Energy	TCA Cycle	-0.01	0.91	0.99



<b>oleate (18:1n9)</b>	Lipid	Long Chain Fatty Acid	0.01	0.91	0.99
<b>epiandrosterone sulfate</b>	Lipid	Steroid	0.03	0.91	0.99
<b>oleamide</b>	Lipid	Fatty Acid, Amide	0.02	0.91	0.99
<b>carnitine</b>	Lipid	Carnitine Metabolism	-0.004	0.92	0.99
<b>2-pyrrolidinone</b>	Xenobiotics	Chemical	-0.02	0.92	0.99
<b>2-keto-3-deoxy-gluconate</b>	Xenobiotics	Food Component/Plant	0.01	0.92	0.99
<b>3-methoxycatechol sulfate (2)</b>	Xenobiotics	Benzoate Metabolism	-0.03	0.92	0.99
<b>phenylalanylglutamate</b>	Peptide	Dipeptide	0.05	0.92	0.99
<b>TL20:3n6 (di-homo-g-linoleic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.01	0.93	0.99
<b>3-[3-(sulfooxy)phenyl]propanoic acid</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.04	0.93	0.99
<b>N-methylpipecolate</b>	Xenobiotics	Chemical	-0.02	0.93	0.99
<b>N-acetyllaiiin</b>	Xenobiotics	Food Component/Plant	0.03	0.93	0.99
<b>deoxycarnitine</b>	Lipid	Carnitine Metabolism	-0.004	0.93	0.99
<b>stearoyl-linoleoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	-0.01	0.93	0.99
<b>HWESASXX*</b>	Peptide	Polypeptide	-0.02	0.93	0.99
<b>3-hydroxydecanoate</b>	Lipid	Fatty Acid, Monohydroxy	0.01	0.93	0.99
<b>1-linoleoyl-GPE (18:2)*</b>	Lipid	Lysolipid	-0.01	0.94	0.99
<b>2-aminophenol sulfate</b>	Xenobiotics	Chemical	-0.02	0.94	0.99
<b>choline</b>	Lipid	Phospholipid Metabolism	-0.004	0.94	0.99
<b>gluconate</b>	Xenobiotics	Food Component/Plant	0.01	0.94	0.99
<b>betonidine</b>	Xenobiotics	Food Component/Plant	0.04	0.94	0.99
<b>aspartylleucine</b>	Peptide	Dipeptide	-0.01	0.94	0.99
<b>l-urobilinogen</b>	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	0.03	0.94	0.99
<b>deoxycholate</b>	Lipid	Secondary Bile Acid Metabolism	-0.01	0.94	0.99
<b>hydroxybutyrylcarnitine*</b>	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.01	0.94	0.99
<b>oleoyl-linoleoyl-glycerophosphocholine (2)*</b>	Lipid	Lysolipid	-0.01	0.94	0.99
<b>hydroxyproline</b>	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.01	0.94	0.99
<b>TL18:4n3 (stearidonic acid)</b>	Lipid	Mole % Total Fatty Acid	0.01	0.94	0.99
<b>N-acetylkynurenine (2)</b>	Amino Acid	Tryptophan Metabolism	0.02	0.94	0.99
<b>pyroglutamylvaline</b>	Peptide	Dipeptide	-0.01	0.94	0.99
<b>cys-gly, oxidized</b>	Amino Acid	Glutathione Metabolism	-0.01	0.95	0.99
<b>pyrraline</b>	Xenobiotics	Food Component/Plant	0.02	0.95	0.99
<b>glycerophosphorylcholine (GPC)</b>	Lipid	Phospholipid Metabolism	0.004	0.95	0.99
<b>TL22:0 (behenic acid)</b>	Lipid	Mole % Total Fatty Acid	0.01	0.95	0.99
<b>palmitoyl-palmitoyl-glycerophosphocholine (2)*</b>	Lipid	Lysolipid	0.01	0.95	0.99

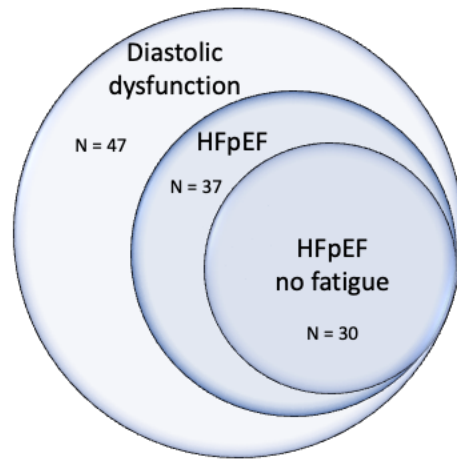
<b>TLTL (Total Total Lipid)</b>	Lipid	Quantitative Total Fatty Acid	0.005	0.95	0.99
<b>pyridoxate</b>	Cofactors and Vitamins	Vitamin B6 Metabolism	0.01	0.95	0.99
<b>linolenate (18:3n3 or 3n6)</b>	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-0.01	0.96	0.99
<b>2-aminoadipate</b>	Amino Acid	Lysine Metabolism	-0.005	0.96	0.99
<b>4-androsten-3alpha,17alpha-diol monosulfate (3)</b>	Lipid	Steroid	-0.01	0.96	0.99
<b>cystine</b>	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.003	0.96	0.99
<b>taurodeoxycholate</b>	Lipid	Secondary Bile Acid Metabolism	0.02	0.96	0.99
<b>TLdm18:0 (plasmalogen stearic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.004	0.96	0.99
<b>palmitoyl-oleoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	-0.004	0.96	0.99
<b>TL16:0 (palmitic acid)</b>	Lipid	Mole % Total Fatty Acid	-0.001	0.96	0.99
<b>scyllo-inositol</b>	Lipid	Inositol Metabolism	0.01	0.96	0.99
<b>2-hydroxyglutarate</b>	Lipid	Fatty Acid, Dicarboxylate	0.004	0.96	0.99
<b>leucylglycine</b>	Peptide	Dipeptide	0.01	0.97	0.99
<b>hypoxanthine</b>	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.01	0.97	0.99
<b>bilirubin</b>	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	0.01	0.97	0.99
<b>sphingosine 1-phosphate</b>	Lipid	Sphingolipid Metabolism	-0.003	0.97	0.99
<b>laurate (12:0)</b>	Lipid	Medium Chain Fatty Acid	0.004	0.97	0.99
<b>ergothioneine</b>	Xenobiotics	Food Component/Plant	0.01	0.97	0.99
<b>1-palmitoyl-GPI* (16:0)*</b>	Lipid	Lysolipid	-0.01	0.97	0.99
<b>N1-Methyl-2-pyridone-5-carboxamide</b>	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.005	0.97	0.99
<b>TL18:0 (stearic acid)</b>	Lipid	Mole % Total Fatty Acid	0.001	0.97	0.99
<b>methyl-4-hydroxybenzoate sulfate</b>	Xenobiotics	Benzoate Metabolism	-0.01	0.97	0.99
<b>5alpha-androstan-3alpha,17beta-diol disulfate</b>	Lipid	Steroid	-0.01	0.97	0.99
<b>4-imidazoleacetate</b>	Amino Acid	Histidine Metabolism	-0.01	0.98	0.99
<b>pipecolate</b>	Amino Acid	Lysine Metabolism	-0.004	0.98	0.99
<b>cinnamoylglycine</b>	Xenobiotics	Food Component/Plant	0.01	0.98	0.99
<b>2-hydroxypalmitate</b>	Lipid	Fatty Acid, Monohydroxy	0.001	0.98	0.99
<b>glycodeoxycholate</b>	Lipid	Secondary Bile Acid Metabolism	0.01	0.98	0.99
<b>3-methylxanthine</b>	Xenobiotics	Xanthine Metabolism	0.01	0.98	0.99
<b>vanillylmandelate (VMA)</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.002	0.98	0.99
<b>4-androsten-3beta,17beta-diol monosulfate (2)</b>	Lipid	Steroid	-0.005	0.98	0.99
<b>gamma-glutamyltyrosine</b>	Peptide	Gamma-glutamyl Amino Acid	-0.001	0.98	0.99

<b>4-hydroxybenzoate</b>	Xenobiotics	Benzoate Metabolism	-0.01	0.98	0.99
<b>palmitoyl-palmitoyl-glycerophosphocholine (1)*</b>	Lipid	Lysolipid	-0.002	0.99	1.00
<b>3-(3-hydroxyphenyl)propionate</b>	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.003	0.99	1.00
<b>3-methyl-2-oxovalerate</b>	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.0005	0.99	1.00
<b>1-stearoyl-GPI (18:0)</b>	Lipid	Lysolipid	0.0002	1.00	1.00
<b>13-methylmyristic acid</b>	Lipid	Fatty Acid, Branched	0.0002	1.00	1.00
<b>cortisone</b>	Lipid	Steroid	0.0001	1.00	1.00

\*Covariates: age, sex, diabetes, hypertension, BMI, and liver fibrosis stage

TCA = tricarboxylic acid cycle; GPE = Glycerophosphoethanolamine; GPC = Glycerophosphocholine; SAM = S-Adenosyl methionine

**Figure S1: Venn diagram showing number of patients meeting each definition of HFpEF and overlap between definitions**



HFpEF = heart failure with preserved ejection fraction

Figure S2: Metabolite missingness

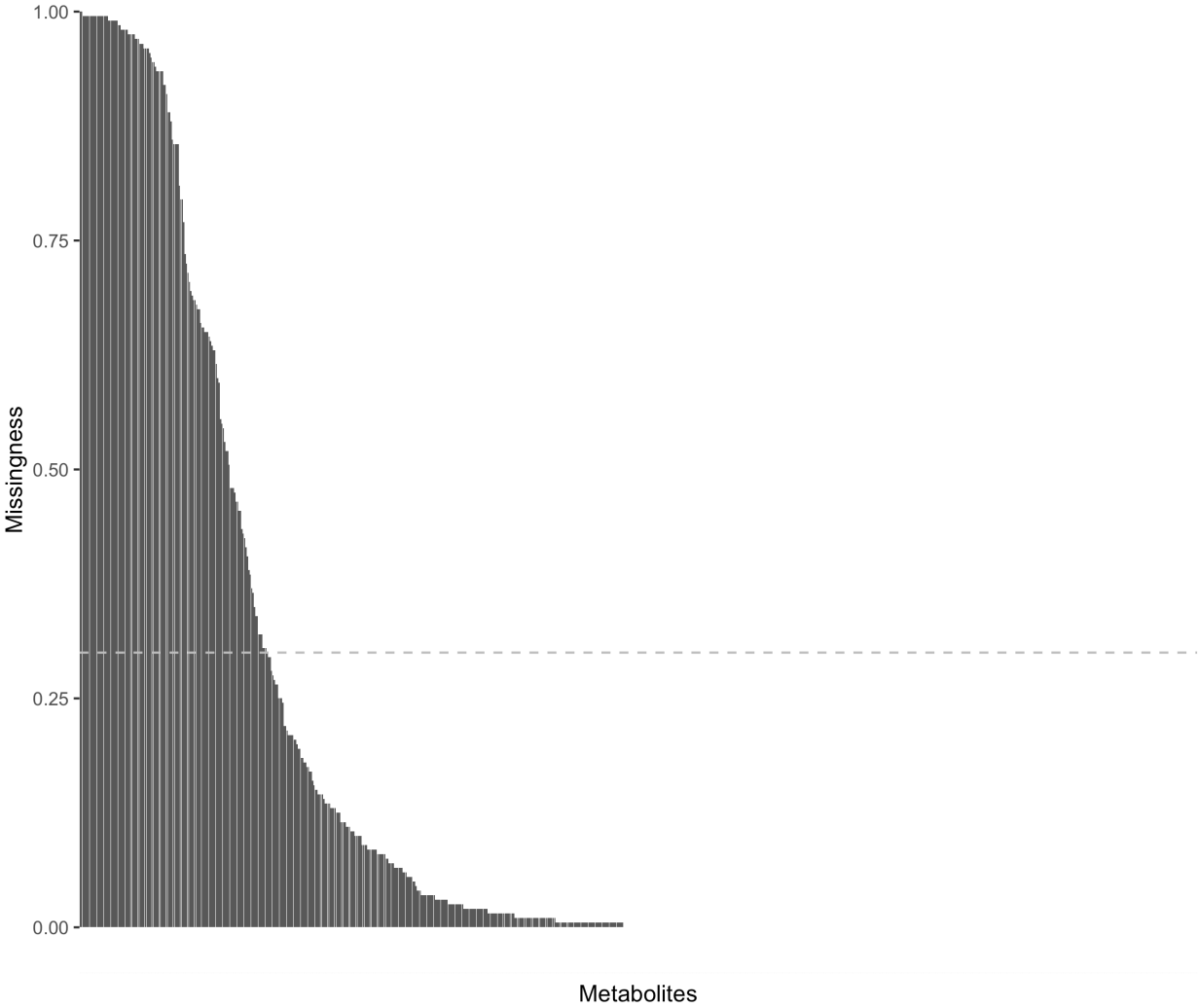
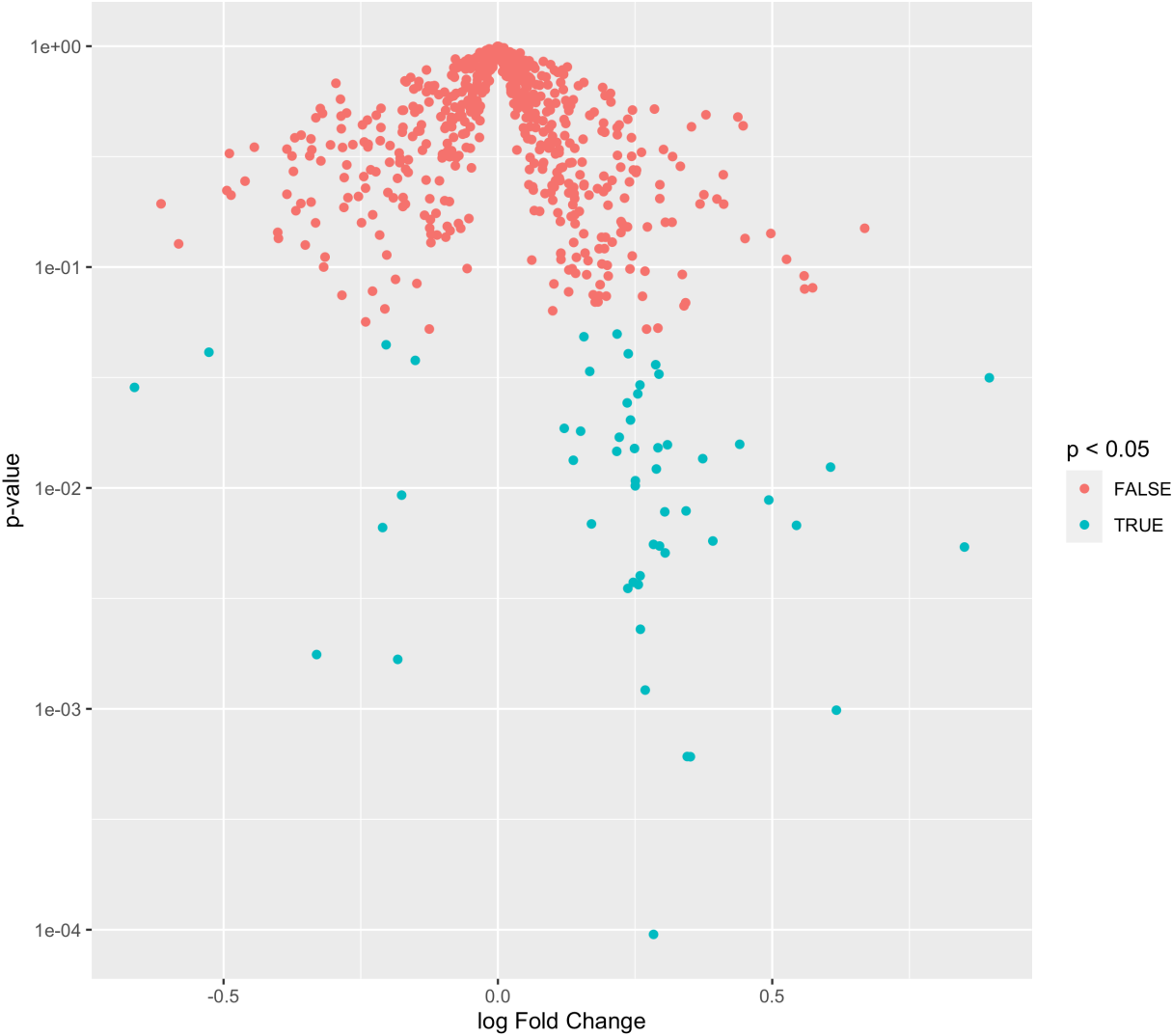
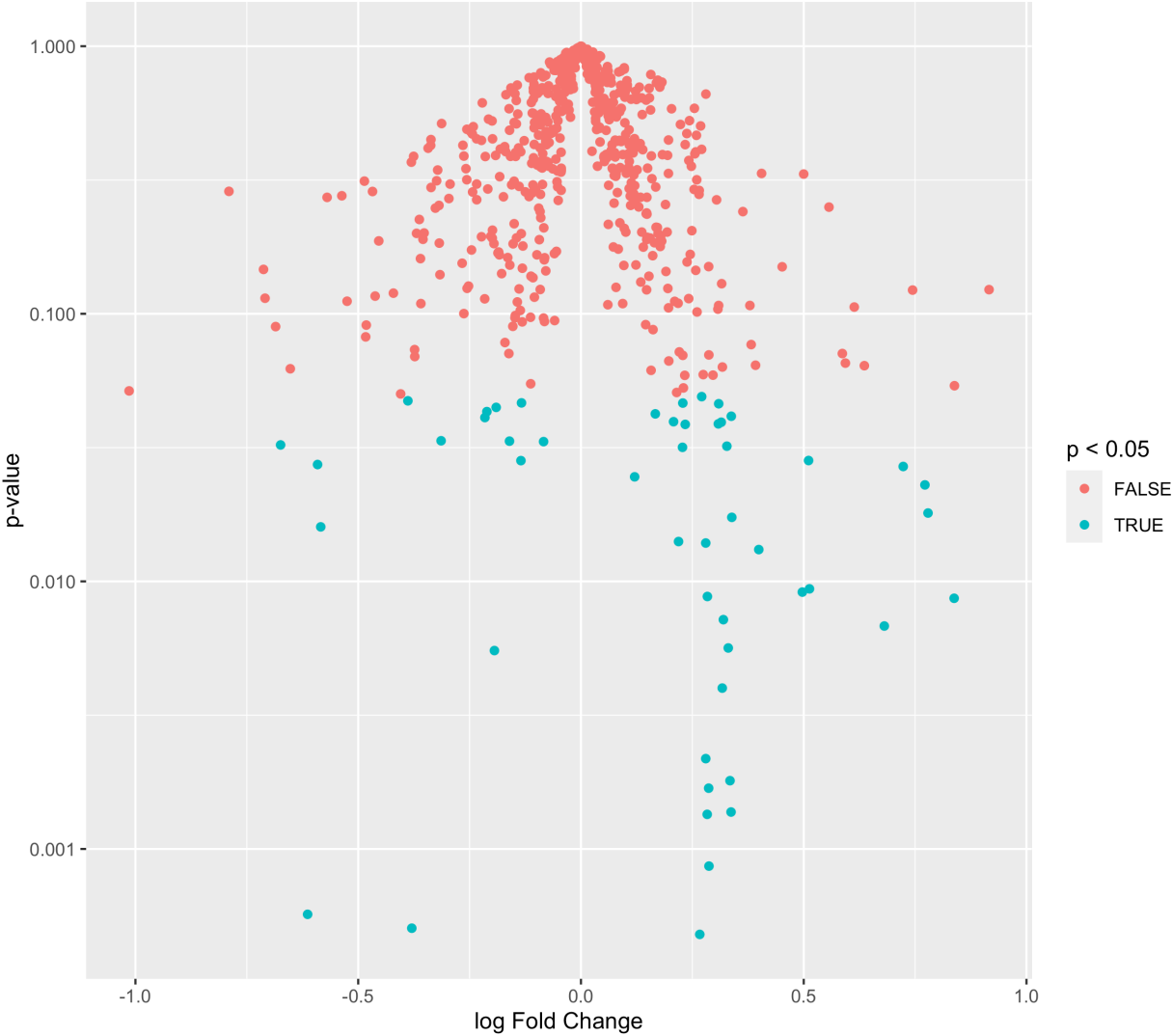


Figure S3: Volcano plot for HFpEF



HFpEF = heart failure with preserved ejection fraction

Figure S4: Volcano plot for HFpEF-no fatigue



HFpEF = heart failure with preserved ejection fraction

Figure S5: Volcano plot for diastolic dysfunction

