

## Supplementary data

**Table S1**

Metabolite VIP	VIP value	Contribution score	p-value	Fold Change	Chemical classes
<b>PE(20:4(5Z,8Z,11Z,14Z)/18:1(11Z))</b>	1.524	2.07	$1.42 \cdot 10^{-3}$	3.428	Phospholipids
<b>PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z))</b>	1.463	1.73	$3.24 \cdot 10^{-3}$	3.738	Phospholipids
<b>Indoleacetic acid</b>	1.450	2.20	$1.77 \cdot 10^{-4}$	2.569	Aromatic compounds-Amines
<b>Hippuric acid</b>	1.435	-2.44	$3.50 \cdot 10^{-6}$	0.056	Amino acids-Derivatives
<b>PE(16:0/20:4(5Z,8Z,11Z,14Z))</b>	1.323	1.93	$3.91 \cdot 10^{-4}$	2.151	Phospholipids
<b>Serotonin</b>	1.317	-2.15	$8.87 \cdot 10^{-6}$	0.476	Amino acids-Derivatives
<b>Cholic acid</b>	1.301	2.01	$3.19 \cdot 10^{-5}$	20.144	Lipids: Fatty acids-Steroids
<b>PC(14:0/16:0)</b>	1.270	1.98	$3.45 \cdot 10^{-5}$	1.566	Phospholipids
<b>Guanidoacetic acid</b>	1.256	1.87	$9.68 \cdot 10^{-5}$	2.290	Amino acids-Derivatives
<b>N-Acetylserotonin</b>	1.255	-1.94	$4.57 \cdot 10^{-5}$	0.377	Amino acids-Derivatives
<b>L-Acetylcarnitine</b>	1.236	1.89	$6.81 \cdot 10^{-5}$	1.531	Lipids: Fatty acids-Steroids
<b>O-Acetyl-L-carnitine</b>	1.233	1.88	$7.14 \cdot 10^{-5}$		Lipids: Fatty acids-Steroids
<b>Glycerophosphocholine</b>	1.229	-1.75	$2.54 \cdot 10^{-4}$	0.425	Lipids: Fatty acids-Steroids
<b>PC(15:0/20:2(11Z,14Z))</b>	1.223	1.82	$1.18 \cdot 10^{-4}$	1.521	Phospholipids
<b>N-acetyltryptophan</b>	1.218	1.79	$1.52 \cdot 10^{-4}$	2.990	Amino acids-Derivatives
<b>4-Trimethylammoniobutanoic acid</b>	1.213	1.82	$1.15 \cdot 10^{-4}$	1.553	Lipids: Fatty acids-Steroids
<b>Trigonelline</b>	1.203	-1.79	$1.39 \cdot 10^{-4}$	0.425	Aromatic compounds-Amines
<b>N-Methyltryptamine</b>	1.192	-1.61	$1.45 \cdot 10^{-3}$	0.323	Aromatic compounds-Amines
<b>Tetradecanoylcarnitine</b>	1.176	1.68	$2.89 \cdot 10^{-4}$	2.052	Lipids: Fatty acids-Steroids
<b>Cytosine</b>	1.164	-1.68	$3.10 \cdot 10^{-4}$	0.601	Nucleotides-Nucleosides-Derivatives
<b>Nicotinic acid</b>	1.152	1.62	$6.80 \cdot 10^{-4}$	1.659	Aromatic compounds-Amines
<b>L-Threonine</b>	1.149	-0.34	>0.05	0.964	Amino acids-Derivatives
<b>Ketoleucine</b>	1.148	-1.60	$7.24 \cdot 10^{-4}$	0.474	Amino acids-Derivatives
<b>PC(15:0/16:0)</b>	1.138	1.57	$5.84 \cdot 10^{-4}$	1.441	Phospholipids
<b>Cholesteryl acetate</b>	1.137	1.56	$1.10 \cdot 10^{-3}$	1.929	Lipids: Fatty acids-Steroids
<b>L-Lysine</b>	1.136	-1.55	$6.95 \cdot 10^{-4}$	0.780	Amino acids-Derivatives
<b>L-Valine</b>	1.128	1.24	$9.30 \cdot 10^{-3}$	1.411	Amino acids-Derivatives
<b>Biotin</b>	1.099	1.49	$8.85 \cdot 10^{-4}$	2.284	Vitamins-Cofactors-Hormones

<b>Uridine</b>	1.084	-1.39	$1.82 \cdot 10^{-3}$	0.671	Nucleotides-Nucleosides-Derivatives
<b>Thiamine monophosphate</b>	1.084	1.42	$2.17 \cdot 10^{-3}$	1.809	Vitamins-Cofactors-Hormones
<b>PC(O-18:2(9Z,12Z)/2:0)</b>	1.081	-1.45	$1.16 \cdot 10^{-3}$	0.843	Phospholipids
<b>Oxoglutaric acid</b>	1.075	1.39	$1.63 \cdot 10^{-3}$	1.702	Organic acids
<b>LysoPC(20:2(11Z,14Z))</b>	1.070	-1.42	$1.37 \cdot 10^{-3}$	0.856	Phospholipids
<b>L-Serine</b>	1.069	0.02	>0.05	1.003	Amino acids-Derivatives
<b>D-Glyceraldehyde-3-phosphate</b>	1.066	-0.14	>0.05		Others
<b>3-(2-Hydroxyphenyl)propanoic acid</b>	1.059	1.39	$1.84 \cdot 10^{-3}$	1.821	Aromatic compounds-Amines
<b>Indole-3-methyl acetate</b>	1.057	-1.39	$1.72 \cdot 10^{-3}$	0.421	Aromatic compounds-Amines
<b>L-Pipeolic acid</b>	1.056	-1.38	$1.86 \cdot 10^{-3}$	0.748	Amino acids-Derivatives
<b>Deoxycytidine</b>	1.052	-1.37	$1.96 \cdot 10^{-3}$	0.671	Nucleotides-Nucleosides-Derivatives
<b>3-Methylhistidine</b>	1.045	-1.35	$2.19 \cdot 10^{-3}$	0.768	Amino acids-Derivatives
<b>N-Alpha-acetyllysine</b>	1.038	-1.34	$2.13 \cdot 10^{-3}$	0.794	Amino acids-Derivatives
<b>Glycocholic acid</b>	1.034	1.22	$4.92 \cdot 10^{-3}$	21.090	Lipids: Fatty acids-Steroids
<b>LysoPC(18:0)</b>	1.016	-1.22	$4.35 \cdot 10^{-3}$	0.857	Phospholipids
<b>Platelet activating factor</b>	1.016	-1.22	$4.50 \cdot 10^{-3}$	0.857	Phospholipids
<b>L-Arginine</b>	1.015	-1.14	$7.97 \cdot 10^{-3}$	0.729	Amino acids-Derivatives
<b>Indoxyl sulfate</b>	1.011	-1.24	$3.61 \cdot 10^{-3}$	0.539	Aromatic compounds-Amines
<b>L-Malic acid</b>	1.008	1.17	$5.88 \cdot 10^{-3}$	1.634	Organic acids
<b>PE(O-16:1(1Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))</b>	1.006	1.10	$1.57 \cdot 10^{-2}$	1.720	Phospholipids
<b>Citramalic acid</b>	0.997	1.23	$3.74 \cdot 10^{-3}$	1.355	Organic acids
<b>Propionylcarnitine</b>	0.995	1.11	$8.34 \cdot 10^{-3}$	1.520	Lipids: Fatty acids-Steroids
<b>PC(18:1(9Z)/18:1(9Z))</b>	0.995	1.22	$3.75 \cdot 10^{-3}$	1.289	Phospholipids
<b>LysoPC(16:0)</b>	0.979	-1.17	$5.30 \cdot 10^{-3}$	0.910	Phospholipids
<b>Stearic acid</b>	0.977	-1.08	$9.25 \cdot 10^{-3}$	0.707	Lipids: Fatty acids-Steroids
<b>Ornithine</b>	0.964	1.03	$1.25 \cdot 10^{-2}$	1.479	Amino acids-Derivatives
<b>Corticosterone</b>	0.960	0.72	>0.05	1.488	Lipids: Fatty acids-Steroids
<b>Uracil</b>	0.958	-1.09	$7.39 \cdot 10^{-3}$	0.706	Nucleotides-Nucleosides-Derivatives
<b>LysoPE(0:0/18:1(11Z))</b>	0.929	0.86	$3.41 \cdot 10^{-2}$	1.434	Phospholipids
<b>PC(16:0/16:0)</b>	0.905	1.00	$1.05 \cdot 10^{-2}$	1.276	Phospholipids
<b>D-Glucose</b>	0.896	-0.77	>0.05	0.806	Sugar
<b>L-Asparagine</b>	0.888	0.96	$1.26 \cdot 10^{-2}$	1.288	Amino acids-Derivatives
<b>PC(20:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))</b>	0.874	-0.86	$2.40 \cdot 10^{-2}$	0.648	Phospholipids
<b>Glucosamine 6-phosphate</b>	0.868	-0.82	$3.09 \cdot 10^{-2}$	0.738	Sugar

<b>L-Glutamine</b>	0.856	0.89	$1.96 \cdot 10^{-2}$	1.186	Amino acids-Derivatives
<b>L-Histidine</b>	0.854	0.88	$1.89 \cdot 10^{-2}$	1.164	Amino acids-Derivatives
<b>Dodecanoylearnitine</b>	0.848	0.89	$1.74 \cdot 10^{-2}$	1.969	Lipids: Fatty acids-Steroids
<b>3-Methylhistamine</b>	0.842	-0.81	$2.77 \cdot 10^{-2}$	0.731	Amino acids-Derivatives
<b>N-Acetyl-L-phenylalanine</b>	0.837	0.78	$3.28 \cdot 10^{-2}$	1.412	Amino acids-Derivatives
<b>Gluconic acid</b>	0.827	-0.81	$3.22 \cdot 10^{-2}$	0.575	Sugar
<b>Alpha-Tocopherol</b>	0.826	0.84	$2.49 \cdot 10^{-2}$	1.203	Lipids: Fatty acids-Steroids
<b>LysoPC(16:1(9Z))</b>	0.826	-0.82	$2.75 \cdot 10^{-2}$	0.839	Phospholipids
<b>Fumaric acid</b>	0.822	0.71	$4.96 \cdot 10^{-2}$	1.424	Organic acids
<b>PC(O-14:1/2:0)</b>	0.813	-0.78	$3.77 \cdot 10^{-2}$	0.828	Phospholipids
<b>Palmitic acid</b>	0.800	-0.74	$3.56 \cdot 10^{-2}$	0.687	Lipids: Fatty acids-Steroids
<b>PC(O-14:0/2:0)</b>	0.791	-0.69	$4.68 \cdot 10^{-2}$	0.908	Phospholipids
<b>3-Hydroxybutyric acid</b>	0.791	0.77	$2.84 \cdot 10^{-2}$	1.379	Organic acids
<b>PC(O-16:1(11Z)/2:0)</b>	0.768	-0.70	$3.89 \cdot 10^{-2}$	0.874	Phospholipids
<b>Azelaic acid</b>	0.764	-0.70	$4.63 \cdot 10^{-2}$	0.756	Lipids: Fatty acids-Steroids
<b>Uric acid</b>	0.761	-0.72	$3.60 \cdot 10^{-2}$	0.759	Nucleotides-Nucleosides-Derivatives
<b>Isocitric acid</b>	0.756	0.70	$4.12 \cdot 10^{-2}$	1.196	Organic acids
<b>LysoPC(20:0)</b>	0.753	-0.52	$1.49 \cdot 10^{-1}$	0.694	Phospholipids
<b>Citric acid</b>	0.748	0.69	$4.38 \cdot 10^{-2}$	1.187	Organic acids
<b>Methylglutaric acid</b>	0.742	-0.66	$4.79 \cdot 10^{-2}$	0.835	Lipids: Fatty acids-Steroids
<b>Phosphorylcholine</b>	0.738	-0.67	$4.35 \cdot 10^{-2}$	0.679	Others
<b>PC(O-18:4/2:0)</b>	0.724	0.64	$4.87 \cdot 10^{-2}$	1.140	Phospholipids
<b>LysoPC(20:3(5Z,8Z,11Z))</b>	0.706	-0.62	$5.48 \cdot 10^{-2}$	0.837	Phospholipids
<b>Linoleic acid</b>	0.673	-0.43	>0.05	0.778	Lipids: Fatty acids-Steroids
<b>Orotic acid</b>	0.662	-0.52	>0.05	0.753	Nucleotides-Nucleosides-Derivatives
<b>PC(15:0/18:2(9Z,12Z))</b>	0.654	0.50	$9.01 \cdot 10^{-2}$	1.031	Phospholipids
<b>trans-Ferulic acid</b>	0.644	-0.39	>0.05	0.504	Others
<b>L-Lactic acid</b>	0.607	-0.45	>0.05	0.928	Organic acids
<b>PC(15:0/20:1(11Z))</b>	0.551	0.38	$1.45 \cdot 10^{-1}$	1.140	Phospholipids
<b>Allantoin</b>	0.532	-0.30	>0.05	0.885	Others
<b>PC(14:0/20:1(11Z))</b>	0.531	0.22	$3.86 \cdot 10^{-1}$	1.105	Phospholipids
<b>Malonate</b>	0.495	0.30	>0.05	1.191	Organic acids
<b>Urocanic acid</b>	0.447	0.03	>0.05	1.037	Amino acids-Derivatives
<b>L-Methionine</b>	0.434	-0.22	>0.05	0.949	Amino acids-Derivatives

**Table S2**

<b>Metabolites VIP</b>	<b>VIP value</b>	<b>Contribution Score</b>	<b>p-value</b>	<b>Fold Change</b>	<b>Chemical classes</b>
<b>PC(O-14:0/2:0)</b>	1.798	-2.785	$3.99 \cdot 10^{-4}$	0.852	Phospholipids
<b>Cytidine</b>	1.596	-2.154	$9.09 \cdot 10^{-4}$	0.803	Nucleotides-Nucleosides-Derivatives
<b>Cytosine</b>	1.455	-1.975	$3.18 \cdot 10^{-3}$	0.754	Nucleotides-Nucleosides-Derivatives
<b>Guanosine</b>	1.380	-1.546	$2.63 \cdot 10^{-3}$	0.602	Nucleotides-Nucleosides-Derivatives
<b>Uric acid</b>	1.377	-1.509	$4.43 \cdot 10^{-3}$	0.777	Nucleotides-Nucleosides-Derivatives
<b>D-Glucose</b>	1.353	1.687	$4.11 \cdot 10^{-2}$	1.329	Sugar
<b>Platelet activating factor</b>	1.343	1.531	>0.1	1.303	Lipids: Fatty acids-Steroids
<b>Caprylic acid</b>	1.297	1.662	$6.04 \cdot 10^{-3}$	2.065	Lipids: Fatty acids-Steroids
<b>L-Lactic acid</b>	1.289	1.459	$1.19 \cdot 10^{-2}$	1.158	Organic acids
<b>Uracil</b>	1.285	-1.366	$6.32 \cdot 10^{-3}$	0.659	Nucleotides-Nucleosides-Derivatives
<b>Propionylcarnitine</b>	1.273	1.373	$9.18 \cdot 10^{-3}$	1.498	Lipids: Fatty acids-Steroids
<b>PC(16:1(9Z)/22:2(13Z,16Z))</b>	1.254	1.250	>0.1	1.095	Phospholipids
<b>Biotin</b>	1.243	-1.488	$6.45 \cdot 10^{-3}$	0.576	Vitamins-Cofactors-Hormones
<b>Uridine</b>	1.234	-1.189	$1.10 \cdot 10^{-2}$	0.662	Nucleotides-Nucleosides-Derivatives
<b>Methylguanidine</b>	1.221	1.193	$1.57 \cdot 10^{-2}$	1.399	Nucleotides-Nucleosides-Derivatives
<b>3-Hydroxybenzoic acid</b>	1.220	-1.223	$7.60 \cdot 10^{-3}$	0.682	Aromatic compounds-Amines
<b>Guanine</b>	1.199	-1.081	$3.33 \cdot 10^{-2}$	0.778	Nucleotides-Nucleosides-Derivatives
<b>LysoPC(18:0)</b>	1.183	1.130	>0.1	1.259	Phospholipids
<b>Inosine</b>	1.181	-1.050	$1.81 \cdot 10^{-2}$	0.768	Nucleotides-Nucleosides-Derivatives
<b>L-Homoserine</b>	1.164	1.352	>0.1	1.202	Amino acids-Derivatives
<b>L-Aspartic acid</b>	1.156	-0.991	$6.69 \cdot 10^{-2}$	0.555	Amino acids-Derivatives
<b>PC(21:0)</b>	1.136	0.892	>0.1	0.984	Phospholipids
<b>Creatine</b>	1.133	1.035	$1.56 \cdot 10^{-2}$	1.195	Amino acids-Derivatives
<b>PC(18:1(9Z)/18:1(9Z))</b>	1.123	1.024	>0.1	1.339	Phospholipids
<b>Cortisol</b>	1.118	1.060	$3.03 \cdot 10^{-2}$	1.557	Lipids: Fatty acids-Steroids
<b>N-Acetylputrescine</b>	1.114	1.373	$2.29 \cdot 10^{-2}$	1.275	Organic acids
<b>Thiamine monophosphate</b>	1.104	-0.904	$6.06 \cdot 10^{-2}$	0.747	Vitamins-Cofactors-Hormones

<b>PC(O-18:2(9Z,12Z)/2:0)</b>	1.095	-0.842	$7.36 \cdot 10^{-2}$	0.759	Phospholipids
<b>L-Arginine</b>	1.087	1.338	>0.1	1.163	Amino acids-Derivatives
<b>4-Trimethylammoniobutanoic acid</b>	1.067	-0.927	$4.71 \cdot 10^{-2}$	0.825	Lipids: Fatty acids-Steroids
<b>L-Threonine</b>	1.064	1.579	>0.1	1.190	Amino acids-Derivatives
<b>Palmitic acid</b>	1.042	-0.829	$1.91 \cdot 10^{-2}$	0.677	Lipids: Fatty acids-Steroids
<b>Hippuric acid</b>	1.035	-0.747	$3.29 \cdot 10^{-2}$	0.494	Amino acids-Derivatives
<b>Ketoleucine</b>	1.029	0.799	$7.47 \cdot 10^{-2}$	0.883	Amino acids-Derivatives
<b>L-Dopa</b>	1.011	1.360	$4.54 \cdot 10^{-2}$	1.273	Vitamins-Cofactors-Hormones
<b>Valerolactone</b>	1.007	-0.823	$3.27 \cdot 10^{-2}$	0.859	Others
<b>PC(14:0/20:1(11Z))</b>	1.005	0.682	>0.1	1.061	Phospholipids
<b>PC(14:0/22:1(13Z))</b>	1.000	0.760	>0.1	1.088	Phospholipids
<b>Adenosine monophosphate</b>	0.998	0.823	>0.1	2.181	Nucleotides-Nucleosides-Derivatives
<b>Urocanic acid</b>	0.991	-0.847	$4.35 \cdot 10^{-2}$	0.448	Amino acids-Derivatives
<b>PC(18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))</b>	0.985	-0.876	>0.1	0.443	Phospholipids
<b>Succinic acid</b>	0.967	-0.785	$7.45 \cdot 10^{-2}$	0.499	Organic acids
<b>NEPSILON,NEPSILON,NEPSILON-TRIMETHYLAMMONIUM</b>	0.956	0.574	>0.1	1.139	Others
<b>LysoPC(18:2(9Z,12Z))</b>	0.953	-0.628	>0.1	0.895	Phospholipids
<b>N-Methyltryptamine</b>	0.945	0.730	>0.1	1.270	Aromatic compounds-Amines
<b>Vanillylmandelic acid</b>	0.941	-0.721	$8.78 \cdot 10^{-2}$	0.376	Aromatic compounds-Amines
<b>Pantothenic acid</b>	0.927	-0.614	$5.47 \cdot 10^{-2}$	0.852	Vitamins-Cofactors-Hormones
<b>Serotonin</b>	0.913	0.475	>0.1	1.356	Amino acids-Derivatives
<b>N-Acetylmethionine</b>	0.911	-1.832	$3.96 \cdot 10^{-2}$	0.617	Amino acids-Derivatives
<b>Picolinic acid</b>	0.908	0.685	>0.1	0.818	Amino acids-Derivatives
<b>SM(d18:1/18:0)</b>	0.908	0.418	>0.1	1.204	Lipids: Fatty acids-Steroids
<b>PC(O-16:1(11Z)/2:0)</b>	0.894	0.671	$9.09 \cdot 10^{-2}$	1.193	Phospholipids
<b>PC(16:0/22:5(4Z,7Z,10Z,13Z,16Z))</b>	0.882	0.371	>0.1	0.989	Phospholipids
<b>L-Serine</b>	0.874	0.978	>0.1	1.190	Amino acids-Derivatives
<b>Pyroglutamic acid</b>	0.873	-0.552	$4.63 \cdot 10^{-2}$	0.845	Amino acids-Derivatives
<b>LysoPC(16:0)</b>	0.867	0.491	>0.1	1.112	Phospholipids
<b>Glyceric acid</b>	0.861	0.784	>0.1	1.043	Sugar
<b>L-Methionine</b>	0.855	0.726	>0.1	1.153	Amino acids-Derivatives
<b>Gluconic acid</b>	0.848	-0.663	$5.10 \cdot 10^{-2}$	0.743	Sugar
<b>Tetradecanoylcarnitine</b>	0.841	-0.581	>0.1	0.755	Lipids: Fatty acids-Steroids
<b>PC(14:1(9Z)/22:2(13Z,16Z))</b>	0.835	0.455	>0.1	0.907	Phospholipids

<b>Caproic acid</b>	0.832	-0.459	>0.1	0.887	Lipids: Fatty acids-Steroids
<b>Diethanolamine</b>	0.831	0.794	>0.1	1.266	Aromatic compounds-Amines
<b>Citric acid</b>	0.818	0.706	>0.1	1.928	Organic acids
<b>Spermidine</b>	0.801	0.648	>0.1	1.012	Aromatic compounds-Amines
<b>Diaminopimelic acid</b>	0.782	0.591	$8.81 \cdot 10^{-2}$	1.339	Amino acids-Derivatives
<b>Menadione</b>	0.773	0.516	>0.1	1.769	Vitamins-Cofactors-Hormones
<b>Isocitric acid</b>	0.748	0.607	>0.1	1.677	Organic acids
<b>Indoleacetic acid</b>	0.739	0.397	>0.1	1.049	Aromatic compounds-Amines
<b>Orotic acid</b>	0.736	-0.332	>0.1	0.739	Nucleotides-Nucleosides-Derivatives
<b>Glucose 1-phosphate</b>	0.733	0.683	>0.1	1.525	Sugar
<b>1-Aminocyclopropanecarboxylic acid</b>	0.722	1.183	>0.1	1.090	Amino acids-Derivatives
<b>5-Hydroxylysine</b>	0.721	2.195	>0.1	1.119	Amino acids-Derivatives
<b>(2E,4E)-2,4-Hexadienoic acid</b>	0.715	0.230	>0.1	1.053	Lipids: Fatty acids-Steroids
<b>3-Aminoisobutanoic acid</b>	0.701	0.527	>0.1	1.023	Amino acids-Derivatives
<b>Glucose 6-phosphate</b>	0.699	0.552	>0.1	2.734	Sugar
<b>Malic acid</b>	0.695	-0.229	>0.1	0.913	Organic acids
<b>Galactitol</b>	0.679	-0.257	>0.1	0.844	Sugar
<b>trans-Cinnamate</b>	0.673	0.743	>0.1	1.090	Aromatic compounds-Amines
<b>Dethiobiotin</b>	0.665	0.280	>0.1	1.175	Lipids: Fatty acids-Steroids
<b>4-Acetamidobutanoic acid</b>	0.652	-0.365	>0.1	0.694	Organic acids
<b>Fumaric acid</b>	0.646	-0.172	>0.1	0.914	Organic acids
<b>Phosphocreatine</b>	0.621	0.454	>0.1	2.010	Amino acids-Derivatives
<b>Decanoylcarnitine</b>	0.617	0.496	>0.1	1.151	Lipids: Fatty acids-Steroids
<b>Riboflavin</b>	0.556	-0.156	>0.1	0.787	Vitamins-Cofactors-Hormones
<b>Deoxycholic acid</b>	0.466	0.357	>0.1	1.076	Lipids: Fatty acids-Steroids
<b>2-Hydroxypyridine</b>	0.440	-0.646	>0.1	0.977	Nucleotides-Nucleosides-Derivatives
<b>Taurine</b>	0.392	0.313	>0.1	1.028	Organic acids

**Table S3**

Elements only in serum :		
	p-value	Fold Change
<b>3-(2-Hydroxyphenyl)propanoic acid</b>	$1.84 \cdot 10^{-3}$	1.821
<b>3-Hydroxybutyric acid</b>	$2.84 \cdot 10^{-2}$	1.379
<b>3-Methylhistamine</b>	$2.77 \cdot 10^{-2}$	0.731
<b>3-Methylhistidine</b>	$2.19 \cdot 10^{-3}$	0.768
<b>Allantoin</b>	>0.05	0.885
<b>Alpha-Tocopherol</b>	$2.49 \cdot 10^{-2}$	1.203
<b>Azelaic acid</b>	$4.63 \cdot 10^{-2}$	0.756
<b>Cholesteryl acetate</b>	$1.10 \cdot 10^{-3}$	1.929
<b>Cholic acid</b>	$3.19 \cdot 10^{-5}$	20.144
<b>Citramalic acid</b>	$3.74 \cdot 10^{-3}$	1.355
<b>Corticosterone</b>	>0.05	1.488
<b>Deoxycytidine</b>	$1.96 \cdot 10^{-3}$	0.671
<b>D-Glyceraldehyde-3-phosphate</b>	>0.05	
<b>Dodecanoylcarnitine</b>	$1.74 \cdot 10^{-2}$	1.969
<b>Glucosamine 6-phosphate</b>	$3.09 \cdot 10^{-2}$	0.738
<b>Glycerophosphocholine</b>	$2.54 \cdot 10^{-4}$	0.425
<b>Glycocholic acid</b>	$4.92 \cdot 10^{-3}$	21.090
<b>Guanidoacetic acid</b>	$9.68 \cdot 10^{-5}$	2.290
<b>Indole-3-methyl acetate</b>	$1.72 \cdot 10^{-3}$	0.421
<b>Indoxyl sulfate</b>	$3.61 \cdot 10^{-3}$	0.539
<b>L-Acetylcarnitine</b>	$6.81 \cdot 10^{-5}$	1.531
<b>L-Asparagine</b>	$1.26 \cdot 10^{-2}$	1.288
<b>L-Glutamine</b>	$1.96 \cdot 10^{-2}$	1.186
<b>L-Histidine</b>	$1.89 \cdot 10^{-2}$	1.164
<b>Linoleic acid</b>	>0.05	0.778
<b>L-Lysine</b>	$6.95 \cdot 10^{-4}$	0.780
<b>L-Pipecolic acid</b>	$1.86 \cdot 10^{-3}$	0.748
<b>L-Valine</b>	$9.30 \cdot 10^{-3}$	1.411
<b>LysoPC(16:1(9Z))</b>	$2.75 \cdot 10^{-2}$	0.839
<b>LysoPC(20:0)</b>	$1.49 \cdot 10^{-1}$	0.694
<b>LysoPC(20:2(11Z,14Z))</b>	$1.37 \cdot 10^{-3}$	0.856
<b>LysoPC(20:3(5Z,8Z,11Z))</b>	$5.48 \cdot 10^{-2}$	0.837
<b>LysoPE(0:0/18:1(11Z))</b>	$3.41 \cdot 10^{-2}$	1.434
<b>Malonate</b>	>0.05	1.191
<b>Methylglutaric acid</b>	$4.79 \cdot 10^{-2}$	0.835

<b>N-Acetyl-L-phenylalanine</b>	$3.28 \cdot 10^{-2}$	1.412
<b>N-Acetylserotonin</b>	$4.57 \cdot 10^{-5}$	0.377
<b>N-acetyltryptophan</b>	$1.52 \cdot 10^{-4}$	2.990
<b>N-Alpha-acetyllysine</b>	$2.13 \cdot 10^{-3}$	0.794
<b>Nicotinic acid</b>	$6.80 \cdot 10^{-4}$	1.659
<b>O-Acetyl-L-carnitine</b>	$7.14 \cdot 10^{-5}$	
<b>Ornithine</b>	$1.25 \cdot 10^{-2}$	1.479
<b>Oxoglutaric acid</b>	$1.63 \cdot 10^{-3}$	1.702
<b>PC(14:0/16:0)</b>	$3.45 \cdot 10^{-5}$	1.566
<b>PC(15:0/16:0)</b>	$5.84 \cdot 10^{-4}$	1.441
<b>PC(15:0/18:2(9Z,12Z))</b>	$9.01 \cdot 10^{-2}$	1.031
<b>PC(15:0/20:1(11Z))</b>	$1.45 \cdot 10^{-1}$	1.140
<b>PC(15:0/20:2(11Z,14Z))</b>	$1.18 \cdot 10^{-4}$	1.521
<b>PC(16:0/16:0)</b>	$1.05 \cdot 10^{-2}$	1.276
<b>PC(20:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))</b>	$2.40 \cdot 10^{-2}$	0.648
<b>PC(O-14:1/2:0)</b>	$4.68 \cdot 10^{-2}$	0.908
<b>PC(O-18:4/2:0)</b>	$4.87 \cdot 10^{-2}$	1.140
<b>PE(16:0/20:4(5Z,8Z,11Z,14Z))</b>	$3.91 \cdot 10^{-4}$	2.151
<b>PE(20:4(5Z,8Z,11Z,14Z)/18:1(11Z))</b>	$1.42 \cdot 10^{-3}$	3.428
<b>PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z))</b>	$3.24 \cdot 10^{-3}$	3.738
<b>PE(O-16:1(1Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))</b>	$1.57 \cdot 10^{-2}$	1.720
<b>Phosphorylcholine</b>	$4.35 \cdot 10^{-2}$	0.679
<b>Stearic acid</b>	$9.25 \cdot 10^{-3}$	0.707
<b>trans-Ferulic acid</b>	>0.05	0.504
<b>Trigonelline</b>	$1.39 \cdot 10^{-4}$	0.425

#### Elements only in soleus :

	p-value	Fold change
<b>(2E,4E)-2,4-Hexadienoic acid</b>	>0.1	1.053
<b>1-Aminocyclopropanecarboxylic acid</b>	>0.1	1.090
<b>2-Hydroxypyridine</b>	>0.1	0.977
<b>3-Aminoisobutanoic acid</b>	>0.1	1.023
<b>3-Hydroxybenzoic acid</b>	$7.60 \cdot 10^{-3}$	0.682
<b>4-Acetamidobutanoic acid</b>	>0.1	0.694
<b>5-Hydroxylysine</b>	>0.1	1.119
<b>Adenosine monophosphate</b>	>0.1	2.181
<b>Caproic acid</b>	>0.1	0.887
<b>Caprylic acid</b>	$6.04 \cdot 10^{-3}$	2.065

Cortisol	$3.03 \cdot 10^{-2}$	1.557
Creatine	$1.56 \cdot 10^{-2}$	1.195
Cytidine	$9.09 \cdot 10^{-4}$	0.803
Decanoylcarnitine	>0.1	1.151
Deoxycholic acid	>0.1	1.076
Dethiobiotin	>0.1	1.175
Diaminopimelic acid	$8.81 \cdot 10^{-2}$	1.339
Diethanolamine	>0.1	1.266
Galactitol	>0.1	0.844
Glucose 1-phosphate	>0.1	1.525
Glucose 6-phosphate	>0.1	2.734
Glyceric acid	>0.1	1.043
Guanine	$3.33 \cdot 10^{-2}$	0.778
Guanosine	$2.63 \cdot 10^{-3}$	0.602
Inosine	$1.81 \cdot 10^{-2}$	0.768
L-Aspartic acid	$6.69 \cdot 10^{-2}$	0.555
L-Dopa	$4.54 \cdot 10^{-2}$	1.273
L-Homoserine	>0.1	1.202
LysoPC(18:2(9Z,12Z))	>0.1	0.895
Menadione	>0.1	1.769
Methylguanidine	$1.57 \cdot 10^{-2}$	1.399
N-Acetylmethionine	$3.96 \cdot 10^{-2}$	0.617
N-Acetylputrescine	$2.29 \cdot 10^{-2}$	1.275
NEPSILON,NEPSILON,NEPSILON-TRIMET	>0.1	1.139
Pantothenic acid	$5.47 \cdot 10^{-2}$	0.852
PC(14:0/22:1(13Z))	>0.1	1.088
PC(14:1(9Z)/22:2(13Z,16Z))	>0.1	0.907
PC(16:0/22:5(4Z,7Z,10Z,13Z,16Z))	>0.1	0.989
PC(16:1(9Z)/22:2(13Z,16Z))	>0.1	1.095
PC(18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	>0.1	0.443
PC(21:0)	>0.1	0.984
Phosphocreatine	>0.1	2.010
Picolinic acid	>0.1	0.818
Pyroglutamic acid	$4.63 \cdot 10^{-2}$	0.845
Riboflavin	>0.1	0.787
SM(d18:1/18:0)	>0.1	1.204
Spermidine	>0.1	1.012
Succinic acid	$7.45 \cdot 10^{-2}$	0.499
Taurine	>0.1	1.028

<b>trans-Cinnamate</b>	>0.1	1.090
<b>Valerolactone</b>	3.27 10 <sup>-2</sup>	0.859
<b>Vanillylmandelic acid</b>	8.78 10 <sup>-2</sup>	0.376

Common elements in serum soleus :	Serum		Soleus	
	p-value	Fold Change	p-value	Fold Change
<b>Biotin</b>	8.85 10 <sup>-4</sup>	2.284	6.45 10 <sup>-3</sup>	0.576
<b>4-Trimethylammoniobutanoic acid</b>	1.15 10 <sup>-4</sup>	1.553	4.71 10 <sup>-2</sup>	0.825
<b>Citric acid</b>	4.38 10 <sup>-2</sup>	1.187	>0.1	1.928
<b>Cytosine</b>	3.10 10 <sup>-4</sup>	0.601	3.18 10 <sup>-3</sup>	0.754
<b>D-Glucose</b>	>0.05	0.806	4.11 10 <sup>-2</sup>	1.329
<b>Fumaric acid</b>	4.96 10 <sup>-2</sup>	1.424	>0.1	0.914
<b>Gluconic acid</b>	3.22 10 <sup>-2</sup>	0.575	5.10 10 <sup>-2</sup>	0.743
<b>Hippuric acid</b>	3.50 10 <sup>-6</sup>	0.056	3.29 10 <sup>-2</sup>	0.494
<b>Indoleacetic acid</b>	1.77 10 <sup>-4</sup>	2.569	>0.1	1.049
<b>Isocitric acid</b>	4.12 10 <sup>-2</sup>	1.196	>0.1	1.677
<b>Ketoleucine</b>	7.24 10 <sup>-4</sup>	0.474	7.47 10 <sup>-2</sup>	0.883
<b>L-Arginine</b>	7.97 10 <sup>-3</sup>	0.729	>0.1	1.163
<b>L-Lactic acid</b>	>0.05	0.928	1.19 10 <sup>-2</sup>	1.158
<b>L-Malic acid</b>	5.88 10 <sup>-3</sup>	1.634	>0.1	0.913
<b>L-Methionine</b>	>0.05	0.949	>0.1	1.153
<b>L-Serine</b>	>0.05	1.003	>0.1	1.190
<b>L-Threonine</b>	>0.05	0.964	>0.1	1.190
<b>LysoPC(16:0)</b>	5.30 10 <sup>-3</sup>	0.910	>0.1	1.112
<b>LysoPC(18:0)</b>	4.35 10 <sup>-3</sup>	0.857	>0.1	1.259
<b>N-Methyltryptamine</b>	1.45 10 <sup>-3</sup>	0.323	>0.1	1.270
<b>Orotic acid</b>	>0.05	0.753	>0.1	0.739
<b>Palmitic acid</b>	3.56 10 <sup>-2</sup>	0.687	1.91 10 <sup>-2</sup>	0.677
<b>PC(14:0/20:1(11Z))</b>	3.86 10 <sup>-1</sup>	1.105	>0.1	1.061
<b>PC(18:1(9Z)/18:1(9Z))</b>	3.75 10 <sup>-3</sup>	1.289	>0.1	1.339
<b>PC(O-14:1/2:0)</b>	3.77 10 <sup>-2</sup>	0.828	3.99 10 <sup>-4</sup>	0.852
<b>PC(O-16:1(11Z)/2:0)</b>	3.89 10 <sup>-2</sup>	0.874	9.09 10 <sup>-2</sup>	1.193
<b>PC(O-18:2(9Z,12Z)/2:0)</b>	1.16 10 <sup>-3</sup>	0.843	7.36 10 <sup>-2</sup>	0.759
<b>Platelet activating factor</b>	4.50 10 <sup>-3</sup>	0.857	>0.1	1.303
<b>Propionylcarnitine</b>	8.34 10 <sup>-3</sup>	1.520	9.18 10 <sup>-3</sup>	1.498
<b>Serotonin</b>	8.87 10 <sup>-6</sup>	0.476	>0.1	1.356
<b>Tetradecanoylcarnitine</b>	2.89 10 <sup>-4</sup>	2.052	>0.1	0.755
<b>Thiamine monophosphate</b>	2.17 10 <sup>-3</sup>	1.809	6.06 10 <sup>-2</sup>	0.747
<b>Uracil</b>	7.39 10 <sup>-3</sup>	0.706	6.32 10 <sup>-3</sup>	0.659

<b>Uric acid</b>	$3.60 \cdot 10^{-2}$	0.759	$4.43 \cdot 10^{-3}$	0.777
<b>Uridine</b>	$1.82 \cdot 10^{-3}$	0.671	$1.10 \cdot 10^{-2}$	0.662
<b>Urocanic acid</b>	>0.05	1.037	$4.35 \cdot 10^{-2}$	0.448