Supplementary Table 3

Fold change, Fold change (log 2) and p-value results of parametric test (t-test) and non-parametric test (Wilcoxon rank-sum test) related to comparison of Tg0 versus WT0 (Results from MetaboAnalyst 3.0)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  |  |  | **Parametric test** | **Nonparametric test** |
|  | **Compound** | **Fold Change** | **Fold Change (log 2)** | **p-value** | **p-value** |
| 1 | Acetylcarnitine | 0.9954 | -0.0067 | 0.9635 | 0.8621 |
| 2 | Acetylcholine | 1.1676 | 0.2236 | 0.0143 | 0.0227 |
| 3 | N-ACETYL-L-ASPARTIC ACID | 1.2211 | 0.2882 | 0.0264 | 0.0339 |
| 4 | N-ACETYLNEURAMINATE | 1.0851 | 0.1179 | 0.0474 | 0.1111 |
| 5 | N1-Acetylspermidine | 1.2097 | 0.2746 | 0.3002 | 0.5538 |
| 6 | ADENINE | 0.6359 | -0.6532 | 0.0585 | 0.0227 |
| 7 | ADENOSINE | 0.7081 | -0.4979 | 0.0051 | 0.0073 |
| 8 | Adrenic acid | 0.8208 | -0.2849 | 0.0002 | 0.0001 |
| 9 | ALANINE | 0.9361 | -0.0953 | 0.1665 | 0.2469 |
| 10 | 4-AMINOBUTANOIC ACID | 0.9943 | -0.0083 | 0.8473 | 0.8621 |
| 11 | L-AMINOCYCLOPROPANE-1-CARBOXYLATE | 0.9908 | -0.0133 | 0.7364 | 0.6511 |
| 12 | 2-AMINOETHYL DIHYDROGEN PHOSPHATE | 1.4343 | 0.5204 | 0.1150 | 0.0585 |
| 13 | 5-AMINOPENTANOATE | 0.8340 | -0.2620 | 0.0185 | 0.0184 |
| 14 | Arachidonic acid ethyl ester | 0.7140 | -0.4861 | 0.0773 | 0.0815 |
| 15 | ARGININE | 0.9571 | -0.0632 | 0.2905 | 0.5079 |
| 16 | Argininosuccinic acid | 1.0132 | 0.0190 | 0.8188 | 0.8078 |
| 17 | AZELAIC ACID | 0.9603 | -0.0584 | 0.6699 | 0.5538 |
| 18 | C16 Sphingosine | 0.8191 | -0.2878 | 0.0965 | 0.1479 |
| 19 | Campesterol | 0.6876 | -0.5403 | 0.0984 | 0.2189 |
| 20 | CARNOSINE | 0.9858 | -0.0207 | 0.8847 | 0.9723 |
| 21 | Cytidine diphosphate choline (CDPcholine) | 1.1486 | 0.1999 | 0.2835 | 0.4221 |
| 22 | Cholesterol | 0.9510 | -0.0725 | 0.1097 | 0.1479 |
| 23 | CITRATE | 0.9886 | -0.0166 | 0.8656 | 0.8621 |
| 24 | CITRULLINE | 1.1571 | 0.2105 | 0.1702 | 0.1285 |
| 25 | CMP | 1.0019 | 0.0027 | 0.9799 | 0.6016 |
| 26 | CREATINE | 0.9938 | -0.0089 | 0.6240 | 0.5538 |
| 27 | CYSTEINE | 1.1352 | 0.1829 | 0.4477 | 0.4221 |
| 28 | Cysteineglutathione disulfide | 1.5549 | 0.6369 | 0.0029 | 0.0018 |
| 29 | CYTIDINE | 0.8599 | -0.2177 | 0.2215 | 0.2189 |
| 30 | CYTOSINE | 0.8440 | -0.2448 | 0.0055 | 0.0018 |
| 31 | D-Aspartic acid | 1.2059 | 0.2701 | 0.0434 | 0.0148 |
| 32 | N-(1-Deoxy-1-fructosyl)alanine | 1.0813 | 0.1127 | 0.1112 | 0.0693 |
| 33 | DEOXYCARNITINE | 1.0487 | 0.0687 | 0.4821 | 0.5079 |
| 34 | DESMOSTEROL | 0.9444 | -0.0825 | 0.0231 | 0.0278 |
| 35 | DG(16:0/18:0/0:0) | 1.0108 | 0.0155 | 0.8316 | 0.7021 |
| 36 | DG(20:2/0:0/22:6) | 1.0338 | 0.0480 | 0.3753 | 0.4639 |
| 37 | DG(22:0/0:0/20:4) | 0.7823 | -0.3543 | 0.3352 | 0.2189 |
| 38 | DG(20:4/24:0/0:0) | 0.7183 | -0.4774 | 0.1240 | 0.1111 |
| 39 | 17,21-DIHYDROXY-4-PREGNENE-3,20-DIONE | 1.2768 | 0.3525 | 0.6240 | 0.9170 |
| 40 | N,N-dimethyl-Safingol | 0.9546 | -0.0671 | 0.6840 | 0.8078 |
| 41 | Docosapentaenoic acid | 0.7738 | -0.3701 | 0.3201 | 0.7021 |
| 42 | Docosatrienoic acid | 0.9412 | -0.0875 | 0.4624 | 0.5079 |
| 43 | Dodecanoic acid | 1.4576 | 0.5436 | 0.0475 | 0.0227 |
| 44 | dUMP | 0.9475 | -0.0778 | 0.0452 | 0.0955 |
| 45 | Eicosatrienoic acid | 0.8565 | -0.2235 | 0.0069 | 0.0148 |
| 46 | Ergothioneine | 1.3438 | 0.4263 | 0.0024 | 0.0056 |
| 47 | 4-O-Galactopyranosylxylose | 0.9059 | -0.1427 | 0.0567 | 0.0491 |
| 48 | GLUTAMIC ACID | 1.0338 | 0.0480 | 0.0317 | 0.0184 |
| 49 | L-GLUTAMINE | 1.0263 | 0.0375 | 0.4431 | 0.5079 |
| 50 | gamma-Glutamylglutamic acid | 1.1838 | 0.2435 | 0.0300 | 0.0227 |
| 51 | GLUTATHIONE | 1.2550 | 0.3277 | 0.0161 | 0.0184 |
| 52 | Glycerophosphocholine | 1.1858 | 0.2459 | 0.1740 | 0.0693 |
| 53 | GLYCINE | 0.9797 | -0.0296 | 0.7829 | 0.6511 |
| 54 | GLYCOCHOLATE | 1.1273 | 0.1729 | 0.7398 | 0.2189 |
| 55 | Guanidylic acid (guanosine monophosphate) | 2.0357 | 1.0255 | 0.0367 | 0.0056 |
| 56 | GUANINE | 1.1510 | 0.2029 | 0.1059 | 0.0815 |
| 57 | Guanosine | 1.0630 | 0.0881 | 0.2282 | 0.4221 |
| 58 | 16-HETE | 0.7226 | -0.4688 | 0.3904 | 0.2773 |
| 59 | HISTIDINE | 1.0397 | 0.0561 | 0.3067 | 0.3824 |
| 60 | Homoanserine | 1.1633 | 0.2183 | 0.0250 | 0.0278 |
| 61 | 14-Hydroperoxy-H4-neuroprostane | 0.8849 | -0.1764 | 0.3083 | 0.3824 |
| 62 | 12-HYDROXYDODECANOIC ACID | 1.0801 | 0.1112 | 0.1793 | 0.3100 |
| 63 | 5-Hydroxyindoleacetic acid | 0.9997 | -0.0004 | 0.9988 | 0.9170 |
| 64 | 13-hydroxyoctadecanoic acid | 0.3873 | -1.3683 | 0.0631 | 0.0955 |
| 65 | HYPOXANTHINE | 0.9995 | -0.0007 | 0.9936 | 1.0000 |
| 66 | INOSINE | 0.9381 | -0.0922 | 0.2599 | 0.2773 |
| 67 | JASMONATE | 1.0904 | 0.1248 | 0.1492 | 0.1930 |
| 68 | LAUROYLCARNITINE | 0.8124 | -0.2997 | 0.1493 | 0.2469 |
| 69 | LEUCINE | 0.9153 | -0.1277 | 0.0111 | 0.0184 |
| 70 | Linolenelaidic acid | 0.9508 | -0.0727 | 0.5264 | 0.6016 |
| 71 | LYSINE | 1.0447 | 0.0631 | 0.1648 | 0.1694 |
| 72 | LysoPA(0:0/16:0) | 0.9791 | -0.0306 | 0.6064 | 0.7021 |
| 73 | LysoPC(14:0/0:0) | 1.1011 | 0.1389 | 0.0020 | 0.0018 |
| 74 | LysoPC(16:1/0:0) | 1.1433 | 0.1932 | 0.0002 | 0.0007 |
| 75 | LysoPC(18:0) | 1.0848 | 0.1174 | 0.0063 | 0.0056 |
| 76 | LysoPC(18:1) | 0.9893 | -0.0156 | 0.6838 | 0.5079 |
| 77 | LysoPC(18:2) | 1.1553 | 0.2082 | 0.0321 | 0.0184 |
| 78 | LysoPC(20:4) | 0.9161 | -0.1264 | 0.0612 | 0.0815 |
| 79 | LysoPC(22:6) | 1.1042 | 0.1430 | 0.0305 | 0.0585 |
| 80 | LysoPE(0:0/20:0) | 0.7322 | -0.4498 | 0.0129 | 0.0278 |
| 81 | LysoPE(0:0/20:1) | 0.9383 | -0.0919 | 0.3752 | 0.3824 |
| 82 | LysoPE(0:0/22:0) | 0.7555 | -0.4046 | 0.0432 | 0.0693 |
| 83 | LysoPE(0:0/22:2) | 1.0929 | 0.1282 | 0.0324 | 0.0693 |
| 84 | LysoPE(15:0/0:0) | 0.8877 | -0.1719 | 0.2583 | 0.5538 |
| 85 | LysoPE(16:1/0:0) | 0.9193 | -0.1214 | 0.2825 | 0.3824 |
| 86 | LysoPE(18:0/0:0) | 1.0017 | 0.0024 | 0.9559 | 0.7544 |
| 87 | LysoPE(22:6/0:0) | 0.9994 | -0.0009 | 0.9674 | 1.0000 |
| 88 | LysoPI(18:0/0:0) | 1.1660 | 0.2215 | 0.0067 | 0.0033 |
| 89 | Lysyl-Leucine | 1.1385 | 0.1871 | 0.0822 | 0.1694 |
| 90 | Lysyl-Proline | 0.5728 | -0.8040 | 0.0254 | 0.0585 |
| 91 | METHACHOLINE | 0.6405 | -0.6427 | 0.1450 | 0.3451 |
| 92 | Methionine | 0.8502 | -0.2342 | 0.0004 | 0.0005 |
| 93 | Methionine sulfoxide | 1.3621 | 0.4458 | 0.0142 | 0.0056 |
| 94 | Methyl linoleate | 0.8283 | -0.2718 | 0.2185 | 0.1694 |
| 95 | Methyladenosine | 1.0571 | 0.0801 | 0.4638 | 0.3824 |
| 96 | 5-Methyldeoxycytidine | 1.2596 | 0.3330 | 0.1545 | 0.0693 |
| 97 | 5'-METHYLTHIOADENOSINE | 1.1342 | 0.1816 | 0.1269 | 0.0491 |
| 98 | MG(0:0/22:6/0:0) | 1.0218 | 0.0311 | 0.4534 | 0.3451 |
| 99 | Myristoylcarnitine | 0.8832 | -0.1791 | 0.1645 | 0.1694 |
| 100 | NICOTINAMIDE | 0.9492 | -0.0752 | 0.4356 | 0.4221 |
| 101 | Octadecanamide | 0.4726 | -1.0812 | 0.0011 | 0.0007 |
| 102 | 9-Octadecenal | 0.9126 | -0.1320 | 0.0376 | 0.0339 |
| 103 | Octadecenoic acid | 1.1969 | 0.2593 | 0.2449 | 0.2469 |
| 104 | Octadecenoylcarnitine | 0.8875 | -0.1723 | 0.1156 | 0.0815 |
| 105 | OCTADECYLPHOSPHOCHOLINE | 0.5925 | -0.7552 | 0.0001 | 0.0003 |
| 106 | Oleamide | 0.5591 | -0.8389 | 0.0026 | 0.0056 |
| 107 | Oleic Acid ethyl ester | 0.5855 | -0.7723 | 0.0404 | 0.0491 |
| 108 | Oleoylglycerophosphoinositol | 1.0758 | 0.1053 | 0.1051 | 0.1285 |
| 109 | L-OLEOYL-RAC-GLYCEROL | 0.9435 | -0.0840 | 0.5425 | 0.6511 |
| 110 | PA(17:0/0:0) | 0.9355 | -0.0962 | 0.9232 | 0.9723 |
| 111 | PA(24:0/21:0) | 0.8771 | -0.1892 | 0.0796 | 0.2469 |
| 112 | Palmitic Acid ethyl ester | 0.8686 | -0.2032 | 0.5275 | 0.4221 |
| 113 | Palmitoyl carnitine | 0.8673 | -0.2054 | 0.1238 | 0.1479 |
| 114 | D-PANTOTHENIC ACID | 0.9171 | -0.1249 | 0.4434 | 0.5538 |
| 115 | PC(16:0/18:2) | 1.1239 | 0.1685 | 0.0162 | 0.0118 |
| 116 | PC(16:0/20:1) | 1.2184 | 0.2850 | 0.0009 | 0.0073 |
| 117 | PC(16:0/22:1) | 1.1408 | 0.1901 | 0.0172 | 0.0278 |
| 118 | PC(18:0/20:4) | 0.9123 | -0.1324 | 0.1501 | 0.2189 |
| 119 | PC(22:0/18:3) | 0.9906 | -0.0136 | 0.9067 | 0.9723 |
| 120 | PC(22:2/20:5) | 0.5226 | -0.9363 | 0.0108 | 0.0409 |
| 121 | PC(22:6/18:2) | 1.0634 | 0.0887 | 0.0893 | 0.0409 |
| 122 | PC(24:1/18:4) | 0.7275 | -0.4590 | 0.0005 | 0.0073 |
| 123 | PE(16:0/0:0) | 1.0622 | 0.0871 | 0.0941 | 0.1285 |
| 124 | PE(16:0/0:0) | 1.0963 | 0.1327 | 0.0490 | 0.0409 |
| 125 | PE(16:0/22:4) | 1.4637 | 0.5497 | 0.0272 | 0.0056 |
| 126 | PE(17:1/0:0) | 0.9333 | -0.0996 | 0.2715 | 0.2469 |
| 127 | PE(18:0/22:2) | 1.0574 | 0.0805 | 0.0998 | 0.0815 |
| 128 | PE(19:1/0:0) | 1.0894 | 0.1236 | 0.0285 | 0.0585 |
| 129 | PE(22:2/20:5) | 1.0397 | 0.0562 | 0.2183 | 0.1479 |
| 130 | PE(22:4/15:0) | 0.8984 | -0.1546 | 0.2198 | 0.3100 |
| 131 | PE(22:6/22:6) | 1.0281 | 0.0400 | 0.4656 | 0.7544 |
| 132 | PE(24:0/22:4) | 1.0809 | 0.1122 | 0.1642 | 0.2189 |
| 133 | PHENACYLAMINE | 0.8671 | -0.2058 | 0.0014 | 0.0073 |
| 134 | PIPECOLINIC ACID | 1.3294 | 0.4108 | 0.2975 | 0.2773 |
| 135 | Propionylcarnitine | 1.2133 | 0.2789 | 0.2396 | 0.3100 |
| 136 | PS(18:1/0:0) | 1.1281 | 0.1738 | 0.1452 | 0.2189 |
| 137 | PS(18:3/20:0) | 1.1431 | 0.1929 | 0.0164 | 0.0339 |
| 138 | PS(18:3/22:0) | 1.0065 | 0.0094 | 0.8469 | 0.9170 |
| 139 | PS(18:4/22:2) | 0.9778 | -0.0323 | 0.9160 | 0.9170 |
| 140 | PS(20:1/20:0) | 0.9082 | -0.1389 | 0.0296 | 0.0585 |
| 141 | PS(20:4/20:0) | 1.0539 | 0.0757 | 0.2090 | 0.2469 |
| 142 | PS(20:4/22:0) | 0.8126 | -0.2994 | 0.0139 | 0.0148 |
| 143 | SERINE | 0.9307 | -0.1037 | 0.1605 | 0.2189 |
| 144 | Spermic acid | 1.2005 | 0.2636 | 0.0728 | 0.0585 |
| 145 | SPERMIDINE | 1.0514 | 0.0723 | 0.6396 | 0.8621 |
| 146 | Sphinganine | 1.0097 | 0.0140 | 0.6881 | 0.7544 |
| 147 | Succinyladenosine | 1.0754 | 0.1048 | 0.1114 | 0.2189 |
| 148 | TAURINE | 1.0571 | 0.0801 | 0.1517 | 0.1930 |
| 149 | TG(14:1/20:5/22:6) | 0.7301 | -0.4539 | 0.0543 | 0.0815 |
| 150 | TG(18:4/18:3/18:4) | 1.1427 | 0.1925 | 0.0321 | 0.0278 |
| 151 | Trihydroxyvitamin D3 | 1.2165 | 0.2827 | 0.0704 | 0.0955 |
| 152 | NE,NE,NE-TRIMETHYLLYSINE | 1.0233 | 0.0333 | 0.6108 | 0.5538 |
| 153 | Uracil | 0.9421 | -0.0860 | 0.3619 | 0.4221 |
| 154 | Urea | 1.2465 | 0.3179 | 0.0000 | 0.0000 |
| 155 | Uric acid |  |  | 1.0000 | 0.7021 |
| 156 | Uridine | 0.9415 | -0.0870 | 0.2518 | 0.3451 |
| 157 | Valyl-Asparagine | 1.0416 | 0.0588 | 0.4030 | 0.4639 |
| 158 | Vitamin A | 0.6495 | -0.6226 | 0.0197 | 0.0093 |
| 159 | XANTHINE | 0.9230 | -0.1156 | 0.1598 | 0.1285 |
| 160 | Cer(18:1/18:0) | 1.0466 | 0.0657 | 0.2392 | 0.8078 |
| 161 | Cer(d18:0/18:1) | 0.8950 | -0.1600 | 0.4898 | 0.4221 |
| 162 | Cer(d18:0/18:1)\_iso2 | 0.9340 | -0.0985 | 0.0467 | 0.1694 |
| 163 | Cer(d18:0/20:0) | 0.8224 | -0.2821 | 0.1976 | 0.2189 |
| 164 | Cer(d18:0/22:0) | 1.1982 | 0.2609 | 0.1205 | 0.1285 |
| 165 | Cer(d18:1/16:0)( N-Palmitoylsphingosine) | 0.8059 | -0.3114 | 0.0030 | 0.0118 |
| 166 | Cer(d18:1/18:1) | 0.9098 | -0.1365 | 0.0422 | 0.0693 |
| 167 | Cer(d18:1/18:1)\_iso2 | 0.8628 | -0.2129 | 0.0005 | 0.0013 |
| 168 | Cer(d18:1/20:0) | 0.9303 | -0.1042 | 0.3608 | 0.5538 |
| 169 | Cer(d18:1/22:1) | 1.6544 | 0.7263 | 0.0064 | 0.0056 |
| 170 | Cer(d18:1/24:1) | 0.9318 | -0.1019 | 0.7021 | 0.9723 |
| 171 | Cer(t18:0/16:0) | 1.2065 | 0.2708 | 0.1345 | 0.1285 |
| 172 | Dihydroceramide | 0.9107 | -0.1350 | 0.0510 | 0.0409 |
| 173 | C2-Dihydroceramide | 1.3335 | 0.4152 | 0.3729 | 0.5079 |
| 174 | HexHexCer(d18:1/18:1) | 1.1564 | 0.2096 | 0.1992 | 0.2189 |
| 175 | HexCer(d18:1/16:0) | 1.0590 | 0.0827 | 0.4163 | 0.6016 |
| 176 | HexCer(d18:1/18:1) | 1.0425 | 0.0601 | 0.3892 | 0.0955 |
| 177 | HexCer(d18:1/20:0) | 0.9503 | -0.0735 | 0.3124 | 0.2469 |
| 178 | HexCer(d18:1/18:0) | 1.1537 | 0.2063 | 0.0002 | 0.0005 |
| 179 | HexCer(d18:1/24:1) | 0.9142 | -0.1294 | 0.7337 | 0.8621 |
| 180 | HexHexCer(d18:1/18:0) | 1.2518 | 0.3240 | 0.0040 | 0.0118 |

Supplementary Table 4

Fold change, Fold change (log 2) and p-value results of parametric test (t-test) and non-parametric test (Wilcoxon rank-sum test) related to comparison of Tg1000 versus Tg0 (Results from MetaboAnalyst 3.0)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  |  |  | **Parametric test** | **Nonparametric test** |
|  | **Compound** | **Fold Change** | **Fold Change(Log 2)** | **p-value** | **p-value** |
| 1 | Acetylcarnitine | 1.0685 | 0.0956 | 0.4907 | 0.3777 |
| 2 | Acetylcholine | 0.8796 | -0.1851 | 0.0326 | 0.0519 |
| 3 | N-ACETYL-L-ASPARTIC ACID | 0.9506 | -0.0730 | 0.4578 | 0.6707 |
| 4 | N-ACETYLNEURAMINATE | 1.0272 | 0.0387 | 0.4918 | 0.5512 |
| 5 | N1-Acetylspermidine | 1.0231 | 0.0329 | 0.9008 | 0.8874 |
| 6 | ADENINE | 1.4270 | 0.5129 | 0.2034 | 0.1782 |
| 7 | ADENOSINE | 0.8390 | -0.2532 | 0.1086 | 0.0887 |
| 8 | Adrenic acid | 1.0550 | 0.0773 | 0.2051 | 0.3777 |
| 9 | ALANINE | 0.9107 | -0.1350 | 0.0610 | 0.0173 |
| 10 | 4-AMINOBUTANOIC ACID | 1.0040 | 0.0058 | 0.8677 | 0.8428 |
| 11 | L-AMINOCYCLOPROPANE-1-CARBOXYLATE | 1.0410 | 0.0580 | 0.1441 | 0.2913 |
| 12 | 2-AMINOETHYL DIHYDROGEN PHOSPHATE | 0.8271 | -0.2738 | 0.2595 | 0.1978 |
| 13 | 5-AMINOPENTANOATE | 1.1441 | 0.1942 | 0.0558 | 0.0597 |
| 14 | Arachidonic acid ethyl ester | 1.1803 | 0.2391 | 0.2235 | 0.1978 |
| 15 | ARGININE | 1.0237 | 0.0337 | 0.4546 | 0.4095 |
| 16 | Argininosuccinic acid | 1.0334 | 0.0474 | 0.5501 | 0.5137 |
| 17 | AZELAIC ACID | 1.1052 | 0.1444 | 0.2688 | 0.0519 |
| 18 | C16 Sphingosine | 1.1791 | 0.2376 | 0.0280 | 0.0205 |
| 19 | Campesterol | 0.3795 | -1.3980 | 0.0209 | 0.0100 |
| 20 | CARNOSINE | 1.0086 | 0.0124 | 0.9183 | 1.0000 |
| 21 | Cytidine diphosphate choline (CDPcholine) | 0.9166 | -0.1256 | 0.4825 | 0.4776 |
| 22 | Cholesterol | 0.9910 | -0.0130 | 0.7234 | 0.7553 |
| 23 | CITRATE | 1.0497 | 0.0700 | 0.4532 | 0.4428 |
| 24 | CITRULLINE | 0.9406 | -0.0884 | 0.4004 | 0.7125 |
| 25 | CMP | 0.9861 | -0.0203 | 0.8320 | 0.9323 |
| 26 | CREATINE | 1.0174 | 0.0248 | 0.2656 | 0.1600 |
| 27 | CYSTEINE | 1.3685 | 0.4526 | 0.0432 | 0.0387 |
| 28 | Cysteineglutathione disulfide | 0.9636 | -0.0536 | 0.7270 | 0.8874 |
| 29 | CYTIDINE | 1.2494 | 0.3213 | 0.0356 | 0.0887 |
| 30 | CYTOSINE | 1.0759 | 0.1055 | 0.2837 | 0.1277 |
| 31 | D-Aspartic acid | 0.9811 | -0.0276 | 0.7886 | 0.8428 |
| 32 | N-(1-Deoxy-1-fructosyl)alanine | 0.9876 | -0.0180 | 0.7627 | 0.7553 |
| 33 | DEOXYCARNITINE | 0.9506 | -0.0731 | 0.4104 | 0.4428 |
| 34 | DESMOSTEROL | 1.0048 | 0.0068 | 0.8478 | 0.8428 |
| 35 | DG(16:0/18:0/0:0) | 1.0286 | 0.0406 | 0.5246 | 0.4776 |
| 36 | DG(20:2/0:0/22:6) | 0.9735 | -0.0387 | 0.4913 | 0.4428 |
| 37 | DG(22:0/0:0/20:4) | 1.1443 | 0.1944 | 0.5751 | 0.5137 |
| 38 | DG(20:4/24:0/0:0) | 1.0485 | 0.0684 | 0.8183 | 0.7553 |
| 39 | 17,21-DIHYDROXY-4-PREGNENE-3,20-DIONE | 0.8411 | -0.2497 | 0.7232 | 0.7988 |
| 40 | N,N-dimethyl-Safingol | 0.9428 | -0.0849 | 0.5554 | 0.6707 |
| 41 | Docosapentaenoic acid | 1.3452 | 0.4278 | 0.0976 | 0.2415 |
| 42 | Docosatrienoic acid | 0.9807 | -0.0282 | 0.7377 | 0.7553 |
| 43 | Dodecanoic acid | 0.9804 | -0.0286 | 0.8734 | 0.8428 |
| 44 | dUMP | 0.9730 | -0.0395 | 0.2128 | 0.3777 |
| 45 | Eicosatrienoic acid | 1.0345 | 0.0489 | 0.5779 | 0.7988 |
| 46 | Ergothioneine | 0.9822 | -0.0259 | 0.8192 | 0.7988 |
| 47 | 4-O-Galactopyranosylxylose | 1.1016 | 0.1396 | 0.0378 | 0.0387 |
| 48 | GLUTAMIC ACID | 1.0002 | 0.0003 | 0.9886 | 0.7125 |
| 49 | L-GLUTAMINE | 1.0791 | 0.1098 | 0.0059 | 0.0023 |
| 50 | gamma-Glutamylglutamic acid | 0.9477 | -0.0775 | 0.3653 | 0.3186 |
| 51 | GLUTATHIONE | 0.8989 | -0.1538 | 0.2845 | 0.1978 |
| 52 | Glycerophosphocholine | 0.9607 | -0.0578 | 0.7634 | 0.7125 |
| 53 | GLYCINE | 1.0685 | 0.0956 | 0.4654 | 0.5899 |
| 54 | GLYCOCHOLATE | 0.8323 | -0.2648 | 0.5666 | 0.1600 |
| 55 | Guanidylic acid (guanosine monophosphate) | 0.5729 | -0.8036 | 0.0131 | 0.0145 |
| 56 | GUANINE | 0.9841 | -0.0231 | 0.8422 | 0.8874 |
| 57 | Guanosine | 0.9110 | -0.1345 | 0.0653 | 0.1135 |
| 58 | 16-HETE | 1.3224 | 0.4031 | 0.3581 | 0.1432 |
| 59 | HISTIDINE | 1.0060 | 0.0086 | 0.8672 | 1.0000 |
| 60 | Homoanserine | 0.9536 | -0.0685 | 0.4022 | 0.5512 |
| 61 | 14-Hydroperoxy-H4-neuroprostane | 0.9815 | -0.0270 | 0.7712 | 0.7553 |
| 62 | 12-HYDROXYDODECANOIC ACID | 0.9646 | -0.0519 | 0.4990 | 0.7553 |
| 63 | 5-Hydroxyindoleacetic acid | 0.8287 | -0.2710 | 0.2723 | 0.2415 |
| 64 | 13-hydroxyoctadecanoic acid | 1.0597 | 0.0836 | 0.9341 | 0.8874 |
| 65 | HYPOXANTHINE | 0.9317 | -0.1021 | 0.2315 | 0.1782 |
| 66 | INOSINE | 0.9623 | -0.0554 | 0.5835 | 0.4776 |
| 67 | JASMONATE | 0.9135 | -0.1305 | 0.0761 | 0.0684 |
| 68 | LAUROYLCARNITINE | 1.0751 | 0.1045 | 0.5928 | 0.9323 |
| 69 | LEUCINE | 1.0143 | 0.0205 | 0.7095 | 0.9774 |
| 70 | Linolenelaidic acid | 0.9289 | -0.1065 | 0.2369 | 0.4095 |
| 71 | LYSINE | 0.9859 | -0.0206 | 0.6595 | 0.6297 |
| 72 | LysoPA(0:0/16:0) | 1.0141 | 0.0202 | 0.6163 | 0.7125 |
| 73 | LysoPC(14:0/0:0) | 0.9736 | -0.0386 | 0.4211 | 0.4776 |
| 74 | LysoPC(16:1/0:0) | 0.9223 | -0.1167 | 0.0285 | 0.0449 |
| 75 | LysoPC(18:0) | 0.9769 | -0.0337 | 0.3953 | 0.3777 |
| 76 | LysoPC(18:1) | 0.9723 | -0.0405 | 0.2369 | 0.1600 |
| 77 | LysoPC(18:2) | 0.9882 | -0.0171 | 0.8441 | 0.9774 |
| 78 | LysoPC(20:4) | 0.9954 | -0.0067 | 0.8969 | 0.7553 |
| 79 | LysoPC(22:6) | 0.9788 | -0.0309 | 0.6266 | 0.8874 |
| 80 | LysoPE(0:0/20:0) | 1.0397 | 0.0561 | 0.7716 | 0.7125 |
| 81 | LysoPE(0:0/20:1) | 1.0001 | 0.0002 | 0.9984 | 0.6707 |
| 82 | LysoPE(0:0/22:0) | 1.1243 | 0.1690 | 0.4464 | 0.6297 |
| 83 | LysoPE(0:0/22:2) | 1.0155 | 0.0222 | 0.6712 | 0.6297 |
| 84 | LysoPE(15:0/0:0) | 0.9860 | -0.0204 | 0.7666 | 0.5899 |
| 85 | LysoPE(16:1/0:0) | 0.9440 | -0.0831 | 0.3763 | 0.6297 |
| 86 | LysoPE(18:0/0:0) | 0.9364 | -0.0948 | 0.0066 | 0.0068 |
| 87 | LysoPE(22:6/0:0) | 0.9938 | -0.0090 | 0.6170 | 0.5137 |
| 88 | LysoPI(18:0/0:0) | 0.9641 | -0.0528 | 0.2880 | 0.3474 |
| 89 | Lysyl-Leucine | 1.0493 | 0.0694 | 0.4160 | 0.2189 |
| 90 | Lysyl-Proline | 1.5448 | 0.6274 | 0.1333 | 0.2415 |
| 91 | METHACHOLINE | 0.6720 | -0.5735 | 0.1057 | 0.0449 |
| 92 | Methionine | 1.0893 | 0.1234 | 0.0907 | 0.1432 |
| 93 | Methionine sulfoxide | 0.9436 | -0.0837 | 0.5824 | 0.5137 |
| 94 | Methyl linoleate | 1.1672 | 0.2230 | 0.1934 | 0.3186 |
| 95 | Methyladenosine | 0.9511 | -0.0724 | 0.4170 | 0.7553 |
| 96 | 5-Methyldeoxycytidine | 1.0184 | 0.0263 | 0.8912 | 0.6297 |
| 97 | 5'-METHYLTHIOADENOSINE | 1.0079 | 0.0114 | 0.8794 | 0.6707 |
| 98 | MG(0:0/22:6/0:0) | 0.9798 | -0.0294 | 0.5245 | 0.8874 |
| 99 | Myristoylcarnitine | 1.0274 | 0.0390 | 0.7332 | 0.8874 |
| 100 | NICOTINAMIDE | 0.8582 | -0.2206 | 0.0415 | 0.0332 |
| 101 | Octadecanamide | 1.1426 | 0.1923 | 0.6025 | 0.8874 |
| 102 | 9-Octadecenal | 1.0557 | 0.0782 | 0.2326 | 0.3777 |
| 103 | Octadecenoic acid | 0.8272 | -0.2738 | 0.2266 | 0.1978 |
| 104 | Octadecenoylcarnitine | 1.0353 | 0.0500 | 0.5996 | 0.6707 |
| 105 | OCTADECYLPHOSPHOCHOLINE | 1.1943 | 0.2562 | 0.1314 | 0.1277 |
| 106 | Oleamide | 1.0405 | 0.0572 | 0.8338 | 0.7553 |
| 107 | Oleic Acid ethyl ester | 1.1392 | 0.1880 | 0.4475 | 0.4776 |
| 108 | Oleoylglycerophosphoinositol | 0.9340 | -0.0985 | 0.0321 | 0.0387 |
| 109 | L-OLEOYL-RAC-GLYCEROL | 0.9969 | -0.0044 | 0.9703 | 1.0000 |
| 110 | PA(17:0/0:0) | 0.8340 | -0.2618 | 0.7690 | 0.8874 |
| 111 | PA(24:0/21:0) | 1.1543 | 0.2070 | 0.0085 | 0.0100 |
| 112 | Palmitic Acid ethyl ester | 1.0814 | 0.1130 | 0.6930 | 0.6707 |
| 113 | Palmitoyl carnitine | 0.9813 | -0.0273 | 0.7947 | 0.9323 |
| 114 | D-PANTOTHENIC ACID | 0.9184 | -0.1228 | 0.4413 | 0.2415 |
| 115 | PC(16:0/18:2) | 1.0622 | 0.0871 | 0.1937 | 0.3186 |
| 116 | PC(16:0/20:1) | 0.9689 | -0.0456 | 0.4305 | 0.1782 |
| 117 | PC(16:0/22:1) | 0.9697 | -0.0444 | 0.4628 | 0.4428 |
| 118 | PC(18:0/20:4) | 1.0234 | 0.0333 | 0.5877 | 0.3777 |
| 119 | PC(22:0/18:3) | 1.1453 | 0.1957 | 0.0957 | 0.1277 |
| 120 | PC(22:2/20:5) | 1.7295 | 0.7904 | 0.0235 | 0.0449 |
| 121 | PC(22:6/18:2) | 1.0428 | 0.0605 | 0.3108 | 0.6297 |
| 122 | PC(24:1/18:4) | 0.9898 | -0.0148 | 0.7530 | 0.6707 |
| 123 | PE(16:0/0:0) | 0.9731 | -0.0394 | 0.4412 | 0.4776 |
| 124 | PE(16:0/0:0) | 0.8825 | -0.1804 | 0.0047 | 0.0023 |
| 125 | PE(16:0/22:4) | 0.8858 | -0.1749 | 0.4648 | 0.1978 |
| 126 | PE(17:1/0:0) | 0.9937 | -0.0091 | 0.9107 | 0.6297 |
| 127 | PE(18:0/22:2) | 0.9997 | -0.0004 | 0.9947 | 0.5899 |
| 128 | PE(19:1/0:0) | 0.9375 | -0.0931 | 0.0714 | 0.1135 |
| 129 | PE(22:2/20:5) | 1.0162 | 0.0232 | 0.5920 | 0.4428 |
| 130 | PE(22:4/15:0) | 0.8959 | -0.1587 | 0.1119 | 0.1978 |
| 131 | PE(22:6/22:6) | 1.0250 | 0.0356 | 0.4253 | 0.5512 |
| 132 | PE(24:0/22:4) | 0.9908 | -0.0134 | 0.8894 | 0.6297 |
| 133 | PHENACYLAMINE | 1.1456 | 0.1961 | 0.0168 | 0.0387 |
| 134 | PIPECOLINIC ACID | 1.1458 | 0.1964 | 0.6522 | 0.5137 |
| 135 | Propionylcarnitine | 1.1832 | 0.2427 | 0.2473 | 0.2415 |
| 136 | PS(18:1/0:0) | 1.0216 | 0.0308 | 0.7900 | 0.9323 |
| 137 | PS(18:3/20:0) | 0.9583 | -0.0614 | 0.3347 | 0.2189 |
| 138 | PS(18:3/22:0) | 0.9850 | -0.0218 | 0.6724 | 0.9323 |
| 139 | PS(18:4/22:2) | 1.1563 | 0.2095 | 0.3917 | 0.5512 |
| 140 | PS(20:1/20:0) | 1.0402 | 0.0569 | 0.2969 | 0.1978 |
| 141 | PS(20:4/20:0) | 0.9092 | -0.1374 | 0.0155 | 0.0387 |
| 142 | PS(20:4/22:0) | 0.9441 | -0.0831 | 0.2681 | 0.2189 |
| 143 | SERINE | 1.0323 | 0.0459 | 0.4777 | 0.7988 |
| 144 | Spermic acid | 1.0304 | 0.0432 | 0.7661 | 0.8874 |
| 145 | SPERMIDINE | 1.1474 | 0.1984 | 0.1849 | 0.1600 |
| 146 | Sphinganine | 1.0199 | 0.0284 | 0.4182 | 0.7988 |
| 147 | Succinyladenosine | 0.8365 | -0.2576 | 0.0202 | 0.0205 |
| 148 | TAURINE | 0.9386 | -0.0914 | 0.0454 | 0.0519 |
| 149 | TG(14:1/20:5/22:6) | 0.9269 | -0.1095 | 0.6173 | 0.4776 |
| 150 | TG(18:4/18:3/18:4) | 0.9226 | -0.1163 | 0.1741 | 0.1978 |
| 151 | Trihydroxyvitamin D3 | 0.8512 | -0.2324 | 0.0956 | 0.1135 |
| 152 | NE,NE,NE-TRIMETHYLLYSINE | 0.9713 | -0.0420 | 0.5154 | 0.5137 |
| 153 | Uracil | 1.0442 | 0.0624 | 0.4878 | 0.4428 |
| 154 | Urea | 1.0110 | 0.0158 | 0.9294 | 0.0387 |
| 155 | Uric acid | 1.1931 | 0.2547 | 0.3228 | 0.2657 |
| 156 | Uridine | 0.9902 | -0.0142 | 0.8081 | 0.9323 |
| 157 | Valyl-Asparagine | 0.9871 | -0.0187 | 0.7189 | 0.6707 |
| 158 | Vitamin A | 1.1560 | 0.2092 | 0.2600 | 0.4095 |
| 159 | XANTHINE | 0.9381 | -0.0922 | 0.2413 | 0.2657 |
| 160 | Cer(18:1/18:0) | 1.0541 | 0.0759 | 0.0493 | 0.0449 |
| 161 | Cer(d18:0/18:1) | 1.2039 | 0.2678 | 0.1382 | 0.0684 |
| 162 | Cer(d18:0/18:1)\_iso2 | 1.0258 | 0.0367 | 0.3222 | 0.3186 |
| 163 | Cer(d18:0/20:0) | 1.0841 | 0.1165 | 0.5091 | 0.4428 |
| 164 | Cer(d18:0/22:0) | 1.0319 | 0.0453 | 0.7869 | 0.5512 |
| 165 | Cer(d18:1/16:0)( N-Palmitoylsphingosine) | 1.1258 | 0.1710 | 0.0770 | 0.1005 |
| 166 | Cer(d18:1/18:1) | 1.0464 | 0.0655 | 0.3819 | 0.2415 |
| 167 | Cer(d18:1/18:1)\_iso2 | 1.0678 | 0.0946 | 0.0310 | 0.0597 |
| 168 | Cer(d18:1/20:0) | 1.0198 | 0.0283 | 0.7223 | 0.7125 |
| 169 | Cer(d18:1/22:1) | 0.9368 | -0.0942 | 0.6449 | 0.7553 |
| 170 | Cer(d18:1/24:1) | 0.9142 | -0.1294 | 0.5146 | 0.5137 |
| 171 | Cer(t18:0/16:0) | 1.1551 | 0.2080 | 0.2758 | 0.2913 |
| 172 | Dihydroceramide | 1.0972 | 0.1338 | 0.1554 | 0.0597 |
| 173 | C2-Dihydroceramide | 0.8404 | -0.2508 | 0.5059 | 0.7988 |
| 174 | HexHexCer(d18:1/18:1) | 1.1213 | 0.1652 | 0.4325 | 0.7988 |
| 175 | HexCer(d18:1/16:0) | 0.9875 | -0.0182 | 0.8720 | 0.7125 |
| 176 | HexCer(d18:1/18:1) | 0.9993 | -0.0010 | 0.9833 | 0.8874 |
| 177 | HexCer(d18:1/20:0) | 0.9949 | -0.0074 | 0.8907 | 0.8874 |
| 178 | HexCer(d18:1/18:0) | 0.9872 | -0.0186 | 0.5890 | 0.6297 |
| 179 | HexCer(d18:1/24:1) | 1.1906 | 0.2516 | 0.4402 | 0.5899 |
| 180 | HexHexCer(d18:1/18:0) | 1.0328 | 0.0466 | 0.6766 | 0.9323 |

Supplementary Table 5

Fold change, Fold change (log 2) and p-value results of parametric test (t-test) and non-parametric test (Wilcoxon rank-sum test) related to comparison of WT1000 versus WT0 (Results from MetaboAnalyst 3.0)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  |  |  | **Parametric test** | **Non-parametric test** |
|  | **Compound** | **Fold Change** | **Fold change (log2)** | **p-value** | **p-value** |
| 1 | Acetylcarnitine | 1.3503 | 0.4333 | 0.1520 | 0.0789 |
| 2 | Acetylcholine | 0.9741 | -0.0378 | 0.6351 | 0.4002 |
| 3 | N-ACETYL-L-ASPARTIC ACID | 0.9602 | -0.0586 | 0.5502 | 0.9048 |
| 4 | N-ACETYLNEURAMINATE | 1.0357 | 0.0506 | 0.5032 | 0.8421 |
| 5 | N1-Acetylspermidine | 1.1995 | 0.2624 | 0.1818 | 0.2428 |
| 6 | ADENINE | 0.9160 | -0.1267 | 0.7005 | 0.5490 |
| 7 | ADENOSINE | 0.9176 | -0.1241 | 0.5753 | 0.9048 |
| 8 | Adrenic acid | 1.1261 | 0.1713 | 0.0892 | 0.1128 |
| 9 | ALANINE | 1.0079 | 0.0114 | 0.8858 | 0.9682 |
| 10 | 4-AMINOBUTANOIC ACID | 1.0191 | 0.0273 | 0.6613 | 0.9048 |
| 11 | L-AMINOCYCLOPROPANE-1-CARBOXYLATE | 1.0171 | 0.0244 | 0.6550 | 0.9682 |
| 12 | 2-AMINOETHYL DIHYDROGEN PHOSPHATE | 1.0679 | 0.0947 | 0.6994 | 0.4470 |
| 13 | 5-AMINOPENTANOATE | 0.9132 | -0.1310 | 0.2215 | 0.2775 |
| 14 | Arachidonic acid ethyl ester | 1.2309 | 0.2997 | 0.2809 | 0.3562 |
| 15 | ARGININE | 0.9627 | -0.0548 | 0.4569 | 0.3562 |
| 16 | Argininosuccinic acid | 0.9630 | -0.0543 | 0.6475 | 0.9048 |
| 17 | AZELAIC ACID | 0.9105 | -0.1353 | 0.2889 | 0.3154 |
| 18 | C16 Sphingosine | 0.8807 | -0.1833 | 0.3264 | 0.3562 |
| 19 | Campesterol | 0.8095 | -0.3048 | 0.3564 | 0.4002 |
| 20 | CARNOSINE | 1.0563 | 0.0790 | 0.5994 | 0.4967 |
| 21 | Cytidine diphosphate choline (CDPcholine) | 0.9456 | -0.0807 | 0.6630 | 0.7802 |
| 22 | Cholesterol | 1.0097 | 0.0139 | 0.7460 | 0.6038 |
| 23 | CITRATE | 0.9523 | -0.0705 | 0.4006 | 0.6607 |
| 24 | CITRULLINE | 1.0094 | 0.0135 | 0.9407 | 0.7197 |
| 25 | CMP | 0.9519 | -0.0711 | 0.5584 | 0.9682 |
| 26 | CREATINE | 1.0145 | 0.0207 | 0.4180 | 0.5490 |
| 27 | CYSTEINE | 1.1670 | 0.2228 | 0.3138 | 0.1564 |
| 28 | Cysteineglutathione disulfide | 1.1204 | 0.1640 | 0.4587 | 0.6607 |
| 29 | CYTIDINE | 1.1610 | 0.2154 | 0.1333 | 0.2775 |
| 30 | CYTOSINE | 1.0785 | 0.1090 | 0.4941 | 0.9048 |
| 31 | D-Aspartic acid | 0.9289 | -0.1064 | 0.3183 | 0.4967 |
| 32 | N-(1-Deoxy-1-fructosyl)alanine | 1.0420 | 0.0593 | 0.5448 | 1.0000 |
| 33 | DEOXYCARNITINE | 1.0708 | 0.0987 | 0.3441 | 0.4470 |
| 34 | DESMOSTEROL | 1.0138 | 0.0197 | 0.7155 | 0.6607 |
| 35 | DG(16:0/18:0/0:0) | 1.0282 | 0.0401 | 0.6947 | 0.7802 |
| 36 | DG(20:2/0:0/22:6) | 1.1026 | 0.1409 | 0.0720 | 0.1333 |
| 37 | DG(22:0/0:0/20:4) | 1.7864 | 0.8371 | 0.0072 | 0.0101 |
| 38 | DG(20:4/24:0/0:0) | 1.5697 | 0.6505 | 0.0159 | 0.0220 |
| 39 | 17,21-DIHYDROXY-4-PREGNENE-3,20-DIONE | 1.3969 | 0.4822 | 0.3681 | 0.4002 |
| 40 | N,N-dimethyl-Safingol | 0.9904 | -0.0139 | 0.9338 | 0.9682 |
| 41 | Docosapentaenoic acid | 1.5752 | 0.6555 | 0.0876 | 0.0947 |
| 42 | Docosatrienoic acid | 0.9454 | -0.0811 | 0.4966 | 0.5490 |
| 43 | Dodecanoic acid | 1.4110 | 0.4968 | 0.1191 | 0.1333 |
| 44 | dUMP | 0.9841 | -0.0231 | 0.5774 | 0.6038 |
| 45 | Eicosatrienoic acid | 0.9709 | -0.0426 | 0.6258 | 0.6607 |
| 46 | Ergothioneine | 1.3078 | 0.3872 | 0.0144 | 0.0101 |
| 47 | 4-O-Galactopyranosylxylose | 1.0897 | 0.1239 | 0.2883 | 0.6038 |
| 48 | GLUTAMIC ACID | 1.0405 | 0.0573 | 0.0928 | 0.0535 |
| 49 | L-GLUTAMINE | 1.0636 | 0.0889 | 0.2531 | 0.3562 |
| 50 | gamma-Glutamylglutamic acid | 1.0815 | 0.1130 | 0.4040 | 0.3562 |
| 51 | GLUTATHIONE | 0.9907 | -0.0135 | 0.9425 | 0.7197 |
| 52 | Glycerophosphocholine | 1.0184 | 0.0263 | 0.9192 | 0.7197 |
| 53 | GLYCINE | 0.9416 | -0.0868 | 0.5747 | 0.6038 |
| 54 | GLYCOCHOLATE | 1.1612 | 0.2156 | 0.1327 | 0.2110 |
| 55 | Guanidylic acid (guanosine monophosphate) | 0.9520 | -0.0709 | 0.9175 | 1.0000 |
| 56 | GUANINE | 1.0297 | 0.0423 | 0.7111 | 0.5490 |
| 57 | Guanosine | 1.0303 | 0.0430 | 0.4622 | 0.9048 |
| 58 | 16-HETE | 0.8226 | -0.2818 | 0.5878 | 0.9682 |
| 59 | HISTIDINE | 1.0780 | 0.1083 | 0.1557 | 0.1564 |
| 60 | Homoanserine | 1.1394 | 0.1882 | 0.1017 | 0.1564 |
| 61 | 14-Hydroperoxy-H4-neuroprostane | 1.6414 | 0.7150 | 0.3253 | 0.1128 |
| 62 | 12-HYDROXYDODECANOIC ACID | 1.1288 | 0.1748 | 0.0433 | 0.0653 |
| 63 | 5-Hydroxyindoleacetic acid | 0.9232 | -0.1152 | 0.6613 | 1.0000 |
| 64 | 13-hydroxyoctadecanoic acid | 1.1079 | 0.1478 | 0.7767 | 0.9048 |
| 65 | HYPOXANTHINE | 0.9542 | -0.0676 | 0.5256 | 0.4002 |
| 66 | INOSINE | 0.8934 | -0.1627 | 0.0949 | 0.0279 |
| 67 | JASMONATE | 1.1102 | 0.1508 | 0.0692 | 0.0535 |
| 68 | LAUROYLCARNITINE | 1.2311 | 0.3000 | 0.2154 | 0.2110 |
| 69 | LEUCINE | 1.0143 | 0.0204 | 0.8265 | 0.6038 |
| 70 | Linolenelaidic acid | 1.0123 | 0.0176 | 0.8849 | 0.8421 |
| 71 | LYSINE | 1.0590 | 0.0826 | 0.4156 | 1.0000 |
| 72 | LysoPA(0:0/16:0) | 0.9767 | -0.0340 | 0.6276 | 0.5490 |
| 73 | LysoPC(14:0/0:0) | 0.9784 | -0.0315 | 0.6037 | 0.4967 |
| 74 | LysoPC(16:1/0:0) | 1.0582 | 0.0816 | 0.2633 | 0.4002 |
| 75 | LysoPC(18:0) | 0.9682 | -0.0466 | 0.5113 | 0.1564 |
| 76 | LysoPC(18:1) | 1.0106 | 0.0152 | 0.8252 | 0.9682 |
| 77 | LysoPC(18:2) | 1.0248 | 0.0354 | 0.7802 | 0.8421 |
| 78 | LysoPC(20:4) | 1.0399 | 0.0565 | 0.6285 | 0.9048 |
| 79 | LysoPC(22:6) | 0.9587 | -0.0609 | 0.5935 | 0.4470 |
| 80 | LysoPE(0:0/20:0) | 0.8035 | -0.3157 | 0.1665 | 0.3154 |
| 81 | LysoPE(0:0/20:1) | 0.9881 | -0.0173 | 0.8652 | 0.9682 |
| 82 | LysoPE(0:0/22:0) | 0.9012 | -0.1501 | 0.5404 | 0.4967 |
| 83 | LysoPE(0:0/22:2) | 1.1062 | 0.1456 | 0.0085 | 0.0101 |
| 84 | LysoPE(15:0/0:0) | 0.8850 | -0.1762 | 0.3263 | 0.6607 |
| 85 | LysoPE(16:1/0:0) | 0.9916 | -0.0122 | 0.9137 | 0.7802 |
| 86 | LysoPE(18:0/0:0) | 1.0283 | 0.0403 | 0.5863 | 1.0000 |
| 87 | LysoPE(22:6/0:0) | 1.0024 | 0.0035 | 0.9097 | 0.7802 |
| 88 | LysoPI(18:0/0:0) | 0.9514 | -0.0719 | 0.3890 | 0.6607 |
| 89 | Lysyl-Leucine | 1.3468 | 0.4295 | 0.0159 | 0.0279 |
| 90 | Lysyl-Proline | 1.0933 | 0.1287 | 0.7512 | 0.9682 |
| 91 | METHACHOLINE | 0.8420 | -0.2481 | 0.6409 | 0.7197 |
| 92 | Methionine | 1.0239 | 0.0341 | 0.7562 | 0.4967 |
| 93 | Methionine sulfoxide | 0.9971 | -0.0042 | 0.9800 | 0.9682 |
| 94 | Methyl linoleate | 1.1528 | 0.2051 | 0.3541 | 0.4002 |
| 95 | Methyladenosine | 0.9352 | -0.0966 | 0.4099 | 0.4002 |
| 96 | 5-Methyldeoxycytidine | 1.3886 | 0.4736 | 0.0196 | 0.0279 |
| 97 | 5'-METHYLTHIOADENOSINE | 0.8206 | -0.2853 | 0.0457 | 0.0220 |
| 98 | MG(0:0/22:6/0:0) | 0.9703 | -0.0435 | 0.5022 | 0.2775 |
| 99 | Myristoylcarnitine | 1.1442 | 0.1944 | 0.1563 | 0.4002 |
| 100 | NICOTINAMIDE | 1.0462 | 0.0652 | 0.5916 | 0.6038 |
| 101 | Octadecanamide | 1.0145 | 0.0208 | 0.9238 | 0.7802 |
| 102 | 9-Octadecenal | 0.9689 | -0.0456 | 0.4476 | 0.3154 |
| 103 | Octadecenoic acid | 1.3992 | 0.4846 | 0.0601 | 0.1823 |
| 104 | Octadecenoylcarnitine | 1.1501 | 0.2018 | 0.1346 | 0.3562 |
| 105 | OCTADECYLPHOSPHOCHOLINE | 1.0748 | 0.1041 | 0.5005 | 1.0000 |
| 106 | Oleamide | 0.8844 | -0.1772 | 0.5088 | 0.4967 |
| 107 | Oleic Acid ethyl ester | 1.2789 | 0.3549 | 0.3049 | 0.3154 |
| 108 | Oleoylglycerophosphoinositol | 1.0035 | 0.0050 | 0.9460 | 0.7197 |
| 109 | L-OLEOYL-RAC-GLYCEROL | 1.1162 | 0.1585 | 0.2010 | 0.2775 |
| 110 | PA(17:0/0:0) | 0.6790 | -0.5585 | 0.6084 | 0.9048 |
| 111 | PA(24:0/21:0) | 0.9965 | -0.0050 | 0.9618 | 0.7802 |
| 112 | Palmitic Acid ethyl ester | 1.2381 | 0.3081 | 0.3222 | 0.3562 |
| 113 | Palmitoyl carnitine | 1.0268 | 0.0382 | 0.8173 | 0.9048 |
| 114 | D-PANTOTHENIC ACID | 0.9412 | -0.0875 | 0.6953 | 0.1333 |
| 115 | PC(16:0/18:2) | 1.0556 | 0.0780 | 0.3343 | 0.3562 |
| 116 | PC(16:0/20:1) | 0.9289 | -0.1064 | 0.2399 | 0.6038 |
| 117 | PC(16:0/22:1) | 0.9238 | -0.1143 | 0.1674 | 0.4002 |
| 118 | PC(18:0/20:4) | 1.0889 | 0.1229 | 0.2377 | 0.1823 |
| 119 | PC(22:0/18:3) | 0.9301 | -0.1046 | 0.4933 | 0.5490 |
| 120 | PC(22:2/20:5) | 1.4154 | 0.5013 | 0.1223 | 0.0947 |
| 121 | PC(22:6/18:2) | 1.0314 | 0.0446 | 0.4293 | 0.3562 |
| 122 | PC(24:1/18:4) | 1.0796 | 0.1105 | 0.4142 | 0.4470 |
| 123 | PE(16:0/0:0) | 1.0298 | 0.0424 | 0.5660 | 0.8421 |
| 124 | PE(16:0/0:0) | 1.0385 | 0.0545 | 0.5495 | 0.8421 |
| 125 | PE(16:0/22:4) | 1.0812 | 0.1126 | 0.4694 | 0.5490 |
| 126 | PE(17:1/0:0) | 1.0530 | 0.0745 | 0.4869 | 0.4470 |
| 127 | PE(18:0/22:2) | 1.0634 | 0.0887 | 0.1788 | 0.2110 |
| 128 | PE(19:1/0:0) | 1.0795 | 0.1104 | 0.2960 | 0.4470 |
| 129 | PE(22:2/20:5) | 1.0994 | 0.1367 | 0.0207 | 0.0279 |
| 130 | PE(22:4/15:0) | 1.0296 | 0.0421 | 0.7231 | 0.4967 |
| 131 | PE(22:6/22:6) | 1.0683 | 0.0954 | 0.1349 | 0.1564 |
| 132 | PE(24:0/22:4) | 0.8749 | -0.1929 | 0.1401 | 0.1128 |
| 133 | PHENACYLAMINE | 1.0843 | 0.1167 | 0.3311 | 0.6607 |
| 134 | PIPECOLINIC ACID | 1.0259 | 0.0369 | 0.9204 | 0.7802 |
| 135 | Propionylcarnitine | 1.0862 | 0.1193 | 0.6764 | 1.0000 |
| 136 | PS(18:1/0:0) | 1.2605 | 0.3340 | 0.0376 | 0.0172 |
| 137 | PS(18:3/20:0) | 1.0472 | 0.0665 | 0.5680 | 0.7802 |
| 138 | PS(18:3/22:0) | 1.0503 | 0.0708 | 0.2945 | 0.4967 |
| 139 | PS(18:4/22:2) | 1.2441 | 0.3151 | 0.2271 | 0.4002 |
| 140 | PS(20:1/20:0) | 0.9843 | -0.0228 | 0.7054 | 0.4967 |
| 141 | PS(20:4/20:0) | 0.9777 | -0.0325 | 0.7119 | 0.5490 |
| 142 | PS(20:4/22:0) | 1.0726 | 0.1011 | 0.4346 | 0.3154 |
| 143 | SERINE | 1.0449 | 0.0633 | 0.6084 | 0.9682 |
| 144 | Spermic acid | 1.2557 | 0.3286 | 0.0644 | 0.0789 |
| 145 | SPERMIDINE | 1.2746 | 0.3500 | 0.1527 | 0.1823 |
| 146 | Sphinganine | 1.0379 | 0.0537 | 0.2897 | 0.4967 |
| 147 | Succinyladenosine | 0.8688 | -0.2029 | 0.1402 | 0.1564 |
| 148 | TAURINE | 1.0309 | 0.0439 | 0.5489 | 0.8421 |
| 149 | TG(14:1/20:5/22:6) | 1.0189 | 0.0270 | 0.9130 | 0.6607 |
| 150 | TG(18:4/18:3/18:4) | 0.9444 | -0.0825 | 0.5726 | 0.6038 |
| 151 | Trihydroxyvitamin D3 | 1.2613 | 0.3349 | 0.0238 | 0.0435 |
| 152 | NE,NE,NE-TRIMETHYLLYSINE | 0.9695 | -0.0447 | 0.6303 | 0.4470 |
| 153 | Uracil | 1.1014 | 0.1394 | 0.1459 | 0.3154 |
| 154 | Urea | 1.1546 | 0.2074 | 0.0057 | 0.0101 |
| 155 | Uric acid | 1.1459 | 0.1965 | 0.7281 | 0.6607 |
| 156 | Uridine | 0.9522 | -0.0707 | 0.4298 | 0.5490 |
| 157 | Valyl-Asparagine | 1.0610 | 0.0854 | 0.6025 | 0.9682 |
| 158 | Vitamin A | 1.2776 | 0.3534 | 0.1656 | 0.2775 |
| 159 | XANTHINE | 0.9908 | -0.0133 | 0.9196 | 0.6038 |
| 160 | Cer(18:1/18:0) | 0.9902 | -0.0142 | 0.8670 | 0.7197 |
| 161 | Cer(d18:0/18:1) | 1.0126 | 0.0180 | 0.9313 | 0.8421 |
| 162 | Cer(d18:0/18:1)\_iso2 | 1.0348 | 0.0493 | 0.4346 | 0.6607 |
| 163 | Cer(d18:0/20:0) | 0.9985 | -0.0022 | 0.9912 | 0.8421 |
| 164 | Cer(d18:0/22:0) | 0.7715 | -0.3743 | 0.0911 | 0.1128 |
| 165 | Cer(d18:1/16:0)( N-Palmitoylsphingosine) | 1.2043 | 0.2682 | 0.1066 | 0.2110 |
| 166 | Cer(d18:1/18:1) | 1.0754 | 0.1049 | 0.1503 | 0.4002 |
| 167 | Cer(d18:1/18:1)\_iso2 | 1.0863 | 0.1195 | 0.1587 | 0.4470 |
| 168 | Cer(d18:1/20:0) | 1.0067 | 0.0096 | 0.9316 | 0.9682 |
| 169 | Cer(d18:1/22:1) | 0.6616 | -0.5960 | 0.0554 | 0.1333 |
| 170 | Cer(d18:1/24:1) | 0.9828 | -0.0251 | 0.9363 | 1.0000 |
| 171 | Cer(t18:0/16:0) | 1.2583 | 0.3315 | 0.1460 | 0.1564 |
| 172 | Dihydroceramide | 1.0640 | 0.0895 | 0.0817 | 0.0653 |
| 173 | C2-Dihydroceramide | 1.1157 | 0.1579 | 0.3653 | 0.2775 |
| 174 | HexHexCer(d18:1/18:1) | 1.2671 | 0.3416 | 0.0386 | 0.0350 |
| 175 | HexCer(d18:1/16:0) | 1.0424 | 0.0599 | 0.5219 | 0.9682 |
| 176 | HexCer(d18:1/18:1) | 1.0278 | 0.0396 | 0.6865 | 0.6038 |
| 177 | HexCer(d18:1/20:0) | 1.0723 | 0.1006 | 0.1785 | 0.4470 |
| 178 | HexCer(d18:1/18:0) | 0.9936 | -0.0093 | 0.8707 | 0.8421 |
| 179 | HexCer(d18:1/24:1) | 0.9179 | -0.1236 | 0.7951 | 0.7802 |
| 180 | HexHexCer(d18:1/18:0) | 1.1205 | 0.1642 | 0.1027 | 0.1823 |