**Table 1. Tg0 versus WT0**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  |  |  | **Parametric test** | **Nonparametric test** |
|  | **Compound** | **Fold Change** | **Fold Change (Log 2)** | **p-value** | **p-value** |
| 1 | Acetylcarnitine | 0.99537 | -0.0067 | 0.96348 | 0.86207 |
| 2 | Acetylcholine | 1.1676 | 0.22359 | 0.014251 | 0.022713 |
| 3 | N-ACETYL-L-ASPARTIC ACID | 1.2211 | 0.28822 | 0.026369 | 0.033865 |
| 4 | N-ACETYLNEURAMINATE | 1.0851 | 0.11785 | 0.047418 | 0.11105 |
| 5 | N1-Acetylspermidine | 1.2097 | 0.27461 | 0.30018 | 0.55379 |
| 6 | ADENINE | 0.63588 | -0.65317 | 0.058542 | 0.022713 |
| 7 | ADENOSINE | 0.70813 | -0.49792 | 0.005114 | 0.007253 |
| 8 | Adrenic acid | 0.8208 | -0.2849 | 0.000177 | 0.000129 |
| 9 | ALANINE | 0.93605 | -0.09534 | 0.16649 | 0.24691 |
| 10 | 4-AMINOBUTANOIC ACID | 0.99428 | -0.00828 | 0.84725 | 0.86207 |
| 11 | L-AMINOCYCLOPROPANE-1-CARBOXYLATE | 0.99084 | -0.01327 | 0.73638 | 0.65105 |
| 12 | 2-AMINOETHYL DIHYDROGEN PHOSPHATE | 1.4343 | 0.52038 | 0.11496 | 0.058483 |
| 13 | 5-AMINOPENTANOATE | 0.83396 | -0.26195 | 0.0185 | 0.018385 |
| 14 | Arachidonic acid ethyl ester | 0.71395 | -0.4861 | 0.077311 | 0.081543 |
| 15 | ARGININE | 0.95712 | -0.06322 | 0.29047 | 0.50788 |
| 16 | Argininosuccinic acid | 1.0132 | 0.018986 | 0.81875 | 0.8078 |
| 17 | AZELAIC ACID | 0.96032 | -0.05841 | 0.66994 | 0.55379 |
| 18 | C16 Sphingosine | 0.81913 | -0.28784 | 0.096485 | 0.14794 |
| 19 | Campesterol | 0.68761 | -0.54034 | 0.098355 | 0.21885 |
| 20 | CARNOSINE | 0.98575 | -0.0207 | 0.88474 | 0.97227 |
| 21 | Cytidine diphosphate choline (CDPcholine) | 1.1486 | 0.19987 | 0.28351 | 0.42211 |
| 22 | Cholesterol | 0.95101 | -0.07247 | 0.10968 | 0.14794 |
| 23 | CITRATE | 0.98858 | -0.01657 | 0.86557 | 0.86207 |
| 24 | CITRULLINE | 1.1571 | 0.21049 | 0.17018 | 0.12853 |
| 25 | CMP | 1.0019 | 0.002693 | 0.97988 | 0.6016 |
| 26 | CREATINE | 0.99382 | -0.00895 | 0.624 | 0.55379 |
| 27 | CYSTEINE | 1.1352 | 0.1829 | 0.44773 | 0.42211 |
| 28 | Cysteineglutathione disulfide | 1.5549 | 0.63686 | 0.002908 | 0.001803 |
| 29 | CYTIDINE | 0.85994 | -0.21769 | 0.22148 | 0.21885 |
| 30 | CYTOSINE | 0.84395 | -0.24477 | 0.005458 | 0.001803 |
| 31 | D-Aspartic acid | 1.2059 | 0.27014 | 0.043376 | 0.014772 |
| 32 | N-(1-Deoxy-1-fructosyl)alanine | 1.0813 | 0.11274 | 0.11122 | 0.069282 |
| 33 | DEOXYCARNITINE | 1.0487 | 0.068662 | 0.48206 | 0.50788 |
| 34 | DESMOSTEROL | 0.94443 | -0.08249 | 0.023066 | 0.027823 |
| 35 | DG(16:0/18:0/0:0) | 1.0108 | 0.015512 | 0.83164 | 0.70209 |
| 36 | DG(20:2/0:0/22:6) | 1.0338 | 0.047972 | 0.37526 | 0.46391 |
| 37 | DG(22:0/0:0/20:4) | 0.78227 | -0.35425 | 0.33521 | 0.21885 |
| 38 | DG(20:4/24:0/0:0) | 0.71827 | -0.4774 | 0.12401 | 0.11105 |
| 39 | 17,21-DIHYDROXY-4-PREGNENE-3,20-DIONE | 1.2768 | 0.3525 | 0.62398 | 0.91701 |
| 40 | N,N-dimethyl-Safingol | 0.95457 | -0.06707 | 0.68395 | 0.8078 |
| 41 | Docosapentaenoic acid | 0.77375 | -0.37006 | 0.32006 | 0.70209 |
| 42 | Docosatrienoic acid | 0.94116 | -0.08749 | 0.46241 | 0.50788 |
| 43 | Dodecanoic acid | 1.4576 | 0.5436 | 0.047482 | 0.022713 |
| 44 | dUMP | 0.94748 | -0.07783 | 0.045206 | 0.095451 |
| 45 | Eicosatrienoic acid | 0.85648 | -0.22351 | 0.006894 | 0.014772 |
| 46 | Ergothioneine | 1.3438 | 0.42627 | 0.002446 | 0.00562 |
| 47 | 4-O-Galactopyranosylxylose | 0.90585 | -0.14265 | 0.056707 | 0.049073 |
| 48 | GLUTAMIC ACID | 1.0338 | 0.047952 | 0.031714 | 0.018385 |
| 49 | L-GLUTAMINE | 1.0263 | 0.037482 | 0.44307 | 0.50788 |
| 50 | gamma-Glutamylglutamic acid | 1.1838 | 0.24346 | 0.030048 | 0.022713 |
| 51 | GLUTATHIONE | 1.255 | 0.32771 | 0.016086 | 0.018385 |
| 52 | Glycerophosphocholine | 1.1858 | 0.24587 | 0.17403 | 0.069282 |
| 53 | GLYCINE | 0.97971 | -0.02958 | 0.7829 | 0.65105 |
| 54 | GLYCOCHOLATE | 1.1273 | 0.17288 | 0.73977 | 0.21885 |
| 55 | Guanidylic acid (guanosine monophosphate) | 2.0357 | 1.0255 | 0.036718 | 0.00562 |
| 56 | GUANINE | 1.151 | 0.2029 | 0.10589 | 0.081543 |
| 57 | Guanosine | 1.063 | 0.088099 | 0.22817 | 0.42211 |
| 58 | 16-HETE | 0.72255 | -0.46884 | 0.39036 | 0.27732 |
| 59 | HISTIDINE | 1.0397 | 0.056144 | 0.30671 | 0.38244 |
| 60 | Homoanserine | 1.1633 | 0.21828 | 0.02498 | 0.027823 |
| 61 | 14-Hydroperoxy-H4-neuroprostane | 0.88493 | -0.17637 | 0.30827 | 0.38244 |
| 62 | 12-HYDROXYDODECANOIC ACID | 1.0801 | 0.11118 | 0.17928 | 0.31003 |
| 63 | 5-Hydroxyindoleacetic acid | 0.9997 | -0.00044 | 0.99875 | 0.91701 |
| 64 | 13-hydroxyoctadecanoic acid | 0.38734 | -1.3683 | 0.063075 | 0.095451 |
| 65 | HYPOXANTHINE | 0.99954 | -0.00066 | 0.99361 | 1 |
| 66 | INOSINE | 0.9381 | -0.09218 | 0.25993 | 0.27732 |
| 67 | JASMONATE | 1.0904 | 0.1248 | 0.14919 | 0.19301 |
| 68 | LAUROYLCARNITINE | 0.81243 | -0.29969 | 0.14931 | 0.24691 |
| 69 | LEUCINE | 0.91527 | -0.12774 | 0.011137 | 0.018385 |
| 70 | Linolenelaidic acid | 0.95084 | -0.07272 | 0.52635 | 0.6016 |
| 71 | LYSINE | 1.0447 | 0.063135 | 0.16479 | 0.16942 |
| 72 | LysoPA(0:0/16:0) | 0.97905 | -0.03055 | 0.60639 | 0.70209 |
| 73 | LysoPC(14:0/0:0) | 1.1011 | 0.13891 | 0.002031 | 0.001803 |
| 74 | LysoPC(16:1/0:0) | 1.1433 | 0.19323 | 0.000192 | 0.00066 |
| 75 | LysoPC(18:0) | 1.0848 | 0.11742 | 0.006322 | 0.00562 |
| 76 | LysoPC(18:1) | 0.98925 | -0.0156 | 0.68384 | 0.50788 |
| 77 | LysoPC(18:2) | 1.1553 | 0.20822 | 0.032117 | 0.018385 |
| 78 | LysoPC(20:4) | 0.91613 | -0.12638 | 0.061157 | 0.081543 |
| 79 | LysoPC(22:6) | 1.1042 | 0.14299 | 0.030459 | 0.058483 |
| 80 | LysoPE(0:0/20:0) | 0.73216 | -0.44978 | 0.01293 | 0.027823 |
| 81 | LysoPE(0:0/20:1) | 0.93831 | -0.09186 | 0.37524 | 0.38244 |
| 82 | LysoPE(0:0/22:0) | 0.75545 | -0.40458 | 0.043209 | 0.069282 |
| 83 | LysoPE(0:0/22:2) | 1.0929 | 0.12815 | 0.032425 | 0.069282 |
| 84 | LysoPE(15:0/0:0) | 0.88766 | -0.17192 | 0.25825 | 0.55379 |
| 85 | LysoPE(16:1/0:0) | 0.91931 | -0.12137 | 0.28253 | 0.38244 |
| 86 | LysoPE(18:0/0:0) | 1.0017 | 0.002384 | 0.9559 | 0.75437 |
| 87 | LysoPE(22:6/0:0) | 0.99937 | -0.00091 | 0.96742 | 1 |
| 88 | LysoPI(18:0/0:0) | 1.166 | 0.22152 | 0.006702 | 0.003259 |
| 89 | Lysyl-Leucine | 1.1385 | 0.1871 | 0.082188 | 0.16942 |
| 90 | Lysyl-Proline | 0.57275 | -0.80402 | 0.02538 | 0.058483 |
| 91 | METHACHOLINE | 0.64054 | -0.64265 | 0.14496 | 0.3451 |
| 92 | Methionine | 0.85018 | -0.23417 | 0.000418 | 0.000456 |
| 93 | Methionine sulfoxide | 1.3621 | 0.44584 | 0.014183 | 0.00562 |
| 94 | Methyl linoleate | 0.82828 | -0.27181 | 0.21846 | 0.16942 |
| 95 | Methyladenosine | 1.0571 | 0.080114 | 0.46381 | 0.38244 |
| 96 | 5-Methyldeoxycytidine | 1.2596 | 0.333 | 0.15452 | 0.069282 |
| 97 | 5'-METHYLTHIOADENOSINE | 1.1342 | 0.18163 | 0.12689 | 0.049073 |
| 98 | MG(0:0/22:6/0:0) | 1.0218 | 0.031097 | 0.45342 | 0.3451 |
| 99 | Myristoylcarnitine | 0.88323 | -0.17914 | 0.16454 | 0.16942 |
| 100 | NICOTINAMIDE | 0.9492 | -0.07522 | 0.43556 | 0.42211 |
| 101 | Octadecanamide | 0.47262 | -1.0812 | 0.001053 | 0.00066 |
| 102 | 9-Octadecenal | 0.91255 | -0.13202 | 0.037573 | 0.033865 |
| 103 | Octadecenoic acid | 1.1969 | 0.25929 | 0.24492 | 0.24691 |
| 104 | Octadecenoylcarnitine | 0.88746 | -0.17225 | 0.11563 | 0.081543 |
| 105 | OCTADECYLPHOSPHOCHOLINE | 0.59245 | -0.75523 | 0.000119 | 0.000306 |
| 106 | Oleamide | 0.55907 | -0.8389 | 0.002648 | 0.00562 |
| 107 | Oleic Acid ethyl ester | 0.58549 | -0.77229 | 0.04042 | 0.049073 |
| 108 | Oleoylglycerophosphoinositol | 1.0758 | 0.10534 | 0.10512 | 0.12853 |
| 109 | L-OLEOYL-RAC-GLYCEROL | 0.94346 | -0.08397 | 0.54251 | 0.65105 |
| 110 | PA(17:0/0:0) | 0.93552 | -0.09616 | 0.92324 | 0.97227 |
| 111 | PA(24:0/21:0) | 0.87712 | -0.18916 | 0.079586 | 0.24691 |
| 112 | Palmitic Acid ethyl ester | 0.8686 | -0.20324 | 0.52749 | 0.42211 |
| 113 | Palmitoyl carnitine | 0.86732 | -0.20537 | 0.1238 | 0.14794 |
| 114 | D-PANTOTHENIC ACID | 0.91709 | -0.12486 | 0.44339 | 0.55379 |
| 115 | PC(16:0/18:2) | 1.1239 | 0.1685 | 0.016218 | 0.011758 |
| 116 | PC(16:0/20:1) | 1.2184 | 0.285 | 0.000856 | 0.007253 |
| 117 | PC(16:0/22:1) | 1.1408 | 0.19006 | 0.017227 | 0.027823 |
| 118 | PC(18:0/20:4) | 0.91231 | -0.1324 | 0.15005 | 0.21885 |
| 119 | PC(22:0/18:3) | 0.99061 | -0.0136 | 0.90669 | 0.97227 |
| 120 | PC(22:2/20:5) | 0.52256 | -0.93633 | 0.010757 | 0.040894 |
| 121 | PC(22:6/18:2) | 1.0634 | 0.088672 | 0.089312 | 0.040894 |
| 122 | PC(24:1/18:4) | 0.72751 | -0.45896 | 0.000537 | 0.007253 |
| 123 | PE(16:0/0:0) | 1.0622 | 0.087075 | 0.094148 | 0.12853 |
| 124 | PE(16:0/0:0) | 1.0963 | 0.1327 | 0.049047 | 0.040894 |
| 125 | PE(16:0/22:4) | 1.4637 | 0.54965 | 0.027226 | 0.00562 |
| 126 | PE(17:1/0:0) | 0.93326 | -0.09965 | 0.27152 | 0.24691 |
| 127 | PE(18:0/22:2) | 1.0574 | 0.080549 | 0.099761 | 0.081543 |
| 128 | PE(19:1/0:0) | 1.0894 | 0.12355 | 0.028543 | 0.058483 |
| 129 | PE(22:2/20:5) | 1.0397 | 0.056192 | 0.21826 | 0.14794 |
| 130 | PE(22:4/15:0) | 0.89837 | -0.15462 | 0.21983 | 0.31003 |
| 131 | PE(22:6/22:6) | 1.0281 | 0.040022 | 0.4656 | 0.75437 |
| 132 | PE(24:0/22:4) | 1.0809 | 0.11217 | 0.16418 | 0.21885 |
| 133 | PHENACYLAMINE | 0.86706 | -0.2058 | 0.001421 | 0.007253 |
| 134 | PIPECOLINIC ACID | 1.3294 | 0.41078 | 0.29745 | 0.27732 |
| 135 | Propionylcarnitine | 1.2133 | 0.2789 | 0.23958 | 0.31003 |
| 136 | PS(18:1/0:0) | 1.1281 | 0.17384 | 0.14519 | 0.21885 |
| 137 | PS(18:3/20:0) | 1.1431 | 0.19294 | 0.01641 | 0.033865 |
| 138 | PS(18:3/22:0) | 1.0065 | 0.009397 | 0.84693 | 0.91701 |
| 139 | PS(18:4/22:2) | 0.97784 | -0.03232 | 0.91602 | 0.91701 |
| 140 | PS(20:1/20:0) | 0.90823 | -0.13887 | 0.029641 | 0.058483 |
| 141 | PS(20:4/20:0) | 1.0539 | 0.075741 | 0.20901 | 0.24691 |
| 142 | PS(20:4/22:0) | 0.81262 | -0.29935 | 0.013891 | 0.014772 |
| 143 | SERINE | 0.93066 | -0.10368 | 0.1605 | 0.21885 |
| 144 | Spermic acid | 1.2005 | 0.2636 | 0.072757 | 0.058483 |
| 145 | SPERMIDINE | 1.0514 | 0.072287 | 0.63964 | 0.86207 |
| 146 | Sphinganine | 1.0097 | 0.013961 | 0.68811 | 0.75437 |
| 147 | Succinyladenosine | 1.0754 | 0.10484 | 0.11135 | 0.21885 |
| 148 | TAURINE | 1.0571 | 0.080142 | 0.15167 | 0.19301 |
| 149 | TG(14:1/20:5/22:6) | 0.73008 | -0.45388 | 0.054295 | 0.081543 |
| 150 | TG(18:4/18:3/18:4) | 1.1427 | 0.19248 | 0.032059 | 0.027823 |
| 151 | Trihydroxyvitamin D3 | 1.2165 | 0.28271 | 0.070399 | 0.095451 |
| 152 | NE,NE,NE-TRIMETHYLLYSINE | 1.0233 | 0.033265 | 0.61076 | 0.55379 |
| 153 | Uracil | 0.94214 | -0.08599 | 0.36191 | 0.42211 |
| 154 | Urea | 1.2465 | 0.31793 | 2.08E-05 | 2.72E-05 |
| 155 | Uric acid |  |  | 1 | 0.70209 |
| 156 | Uridine | 0.9415 | -0.08697 | 0.25178 | 0.3451 |
| 157 | Valyl-Asparagine | 1.0416 | 0.058807 | 0.40296 | 0.46391 |
| 158 | Vitamin A | 0.6495 | -0.62259 | 0.019671 | 0.009288 |
| 159 | XANTHINE | 0.92302 | -0.11557 | 0.15975 | 0.12853 |
| 160 | Cer(18:1/18:0) | 1.0466 | 0.065728 | 0.23917 | 0.8078 |
| 161 | Cer(d18:0/18:1) | 0.89504 | -0.15997 | 0.48978 | 0.42211 |
| 162 | Cer(d18:0/18:1)\_iso2 | 0.93401 | -0.09849 | 0.046707 | 0.16942 |
| 163 | Cer(d18:0/20:0) | 0.82239 | -0.2821 | 0.19757 | 0.21885 |
| 164 | Cer(d18:0/22:0) | 1.1982 | 0.26091 | 0.12054 | 0.12853 |
| 165 | Cer(d18:1/16:0)( N-Palmitoylsphingosine) | 0.80589 | -0.31135 | 0.003028 | 0.011758 |
| 166 | Cer(d18:1/18:1) | 0.90976 | -0.13645 | 0.04217 | 0.069282 |
| 167 | Cer(d18:1/18:1)\_iso2 | 0.86278 | -0.21294 | 0.00051 | 0.001306 |
| 168 | Cer(d18:1/20:0) | 0.93032 | -0.1042 | 0.36081 | 0.55379 |
| 169 | Cer(d18:1/22:1) | 1.6544 | 0.72631 | 0.006368 | 0.00562 |
| 170 | Cer(d18:1/24:1) | 0.93181 | -0.10189 | 0.70206 | 0.97227 |
| 171 | Cer(t18:0/16:0) | 1.2065 | 0.27078 | 0.13445 | 0.12853 |
| 172 | Dihydroceramide | 0.91066 | -0.13502 | 0.05104 | 0.040894 |
| 173 | C2-Dihydroceramide | 1.3335 | 0.41522 | 0.37294 | 0.50788 |
| 174 | HexHexCer(d18:1/18:1) | 1.1564 | 0.20964 | 0.19917 | 0.21885 |
| 175 | HexCer(d18:1/16:0) | 1.059 | 0.082703 | 0.41631 | 0.6016 |
| 176 | HexCer(d18:1/18:1) | 1.0425 | 0.060099 | 0.38924 | 0.095451 |
| 177 | HexCer(d18:1/20:0) | 0.95033 | -0.07349 | 0.31238 | 0.24691 |
| 178 | HexCer(d18:1/18:0) | 1.1537 | 0.20625 | 0.000167 | 0.000456 |
| 179 | HexCer(d18:1/24:1) | 0.91421 | -0.12941 | 0.73365 | 0.86207 |
| 180 | HexHexCer(d18:1/18:0) | 1.2518 | 0.324 | 0.004044 | 0.011758 |

**Table 2. Tg1000 versus Tg0**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  |  |  | **Parametric test** | **Nonparametric test** |
|  | **Compound** | **Fold Change** | **Fold Change(Log 2)** | **p-value** | **p-value** |
| 1 | Acetylcarnitine | 1.0685 | 0.095585 | 0.49065 | 0.37769 |
| 2 | Acetylcholine | 0.8796 | -0.18509 | 0.032611 | 0.051865 |
| 3 | N-ACETYL-L-ASPARTIC ACID | 0.95064 | -0.073032 | 0.45783 | 0.67066 |
| 4 | N-ACETYLNEURAMINATE | 1.0272 | 0.038725 | 0.49181 | 0.55117 |
| 5 | N1-Acetylspermidine | 1.0231 | 0.032944 | 0.9008 | 0.88739 |
| 6 | ADENINE | 1.427 | 0.51294 | 0.20343 | 0.17818 |
| 7 | ADENOSINE | 0.83902 | -0.25322 | 0.10855 | 0.088734 |
| 8 | Adrenic acid | 1.055 | 0.077275 | 0.20505 | 0.37769 |
| 9 | ALANINE | 0.91068 | -0.13498 | 0.06098 | 0.017271 |
| 10 | 4-AMINOBUTANOIC ACID | 1.004 | 0.0057912 | 0.86765 | 0.84284 |
| 11 | L-AMINOCYCLOPROPANE-1-CARBOXYLATE | 1.041 | 0.057993 | 0.14408 | 0.29134 |
| 12 | 2-AMINOETHYL DIHYDROGEN PHOSPHATE | 0.82714 | -0.2738 | 0.25947 | 0.19781 |
| 13 | 5-AMINOPENTANOATE | 1.1441 | 0.19423 | 0.05577 | 0.059657 |
| 14 | Arachidonic acid ethyl ester | 1.1803 | 0.23914 | 0.22349 | 0.19781 |
| 15 | ARGININE | 1.0237 | 0.033738 | 0.45461 | 0.40951 |
| 16 | Argininosuccinic acid | 1.0334 | 0.047405 | 0.55013 | 0.51372 |
| 17 | AZELAIC ACID | 1.1052 | 0.14435 | 0.26877 | 0.051865 |
| 18 | C16 Sphingosine | 1.1791 | 0.23763 | 0.027984 | 0.020489 |
| 19 | Campesterol | 0.37946 | -1.398 | 0.020946 | 0.010029 |
| 20 | CARNOSINE | 1.0086 | 0.012392 | 0.91833 | 1 |
| 21 | Cytidine diphosphate choline (CDPcholine) | 0.91662 | -0.12561 | 0.48248 | 0.47758 |
| 22 | Cholesterol | 0.99101 | -0.013026 | 0.72338 | 0.75528 |
| 23 | CITRATE | 1.0497 | 0.07002 | 0.4532 | 0.44283 |
| 24 | CITRULLINE | 0.94058 | -0.088379 | 0.40039 | 0.71254 |
| 25 | CMP | 0.98606 | -0.02025 | 0.83195 | 0.9323 |
| 26 | CREATINE | 1.0174 | 0.024844 | 0.26557 | 0.15997 |
| 27 | CYSTEINE | 1.3685 | 0.45256 | 0.043229 | 0.038721 |
| 28 | Cysteineglutathione disulfide | 0.96356 | -0.053551 | 0.72699 | 0.88739 |
| 29 | CYTIDINE | 1.2494 | 0.32127 | 0.035646 | 0.088734 |
| 30 | CYTOSINE | 1.0759 | 0.10551 | 0.28373 | 0.12769 |
| 31 | D-Aspartic acid | 0.98107 | -0.027572 | 0.78857 | 0.84284 |
| 32 | N-(1-Deoxy-1-fructosyl)alanine | 0.98761 | -0.01799 | 0.76265 | 0.75528 |
| 33 | DEOXYCARNITINE | 0.95062 | -0.073058 | 0.41039 | 0.44283 |
| 34 | DESMOSTEROL | 1.0048 | 0.0068392 | 0.84782 | 0.84284 |
| 35 | DG(16:0/18:0/0:0) | 1.0286 | 0.040636 | 0.52458 | 0.47758 |
| 36 | DG(20:2/0:0/22:6) | 0.97352 | -0.038715 | 0.49127 | 0.44283 |
| 37 | DG(22:0/0:0/20:4) | 1.1443 | 0.19441 | 0.57514 | 0.51372 |
| 38 | DG(20:4/24:0/0:0) | 1.0485 | 0.06837 | 0.81825 | 0.75528 |
| 39 | 17,21-DIHYDROXY-4-PREGNENE-3,20-DIONE | 0.84107 | -0.2497 | 0.7232 | 0.79875 |
| 40 | N,N-dimethyl-Safingol | 0.94283 | -0.084937 | 0.55539 | 0.67066 |
| 41 | Docosapentaenoic acid | 1.3452 | 0.42784 | 0.097601 | 0.24152 |
| 42 | Docosatrienoic acid | 0.98066 | -0.028177 | 0.73768 | 0.75528 |
| 43 | Dodecanoic acid | 0.98035 | -0.028632 | 0.87341 | 0.84284 |
| 44 | dUMP | 0.97301 | -0.039477 | 0.21282 | 0.37769 |
| 45 | Eicosatrienoic acid | 1.0345 | 0.048881 | 0.57789 | 0.79875 |
| 46 | Ergothioneine | 0.98219 | -0.025929 | 0.81918 | 0.79875 |
| 47 | 4-O-Galactopyranosylxylose | 1.1016 | 0.13956 | 0.037788 | 0.038721 |
| 48 | GLUTAMIC ACID | 1.0002 | 0.00034957 | 0.9886 | 0.71254 |
| 49 | L-GLUTAMINE | 1.0791 | 0.10977 | 0.005948 | 0.002316 |
| 50 | gamma-Glutamylglutamic acid | 0.94773 | -0.077457 | 0.3653 | 0.31859 |
| 51 | GLUTATHIONE | 0.89888 | -0.15379 | 0.28451 | 0.19781 |
| 52 | Glycerophosphocholine | 0.96072 | -0.057809 | 0.76342 | 0.71254 |
| 53 | GLYCINE | 1.0685 | 0.095554 | 0.46539 | 0.58988 |
| 54 | GLYCOCHOLATE | 0.8323 | -0.26482 | 0.56662 | 0.15997 |
| 55 | Guanidylic acid (guanosine monophosphate) | 0.57293 | -0.80357 | 0.013121 | 0.014493 |
| 56 | GUANINE | 0.98412 | -0.023096 | 0.84221 | 0.88739 |
| 57 | Guanosine | 0.911 | -0.13447 | 0.065293 | 0.1135 |
| 58 | 16-HETE | 1.3224 | 0.40312 | 0.35807 | 0.14317 |
| 59 | HISTIDINE | 1.006 | 0.0086448 | 0.86717 | 1 |
| 60 | Homoanserine | 0.95363 | -0.068493 | 0.40219 | 0.55117 |
| 61 | 14-Hydroperoxy-H4-neuroprostane | 0.98148 | -0.026971 | 0.77116 | 0.75528 |
| 62 | 12-HYDROXYDODECANOIC ACID | 0.96464 | -0.051936 | 0.49897 | 0.75528 |
| 63 | 5-Hydroxyindoleacetic acid | 0.82873 | -0.27103 | 0.27232 | 0.24152 |
| 64 | 13-hydroxyoctadecanoic acid | 1.0597 | 0.083626 | 0.93409 | 0.88739 |
| 65 | HYPOXANTHINE | 0.93166 | -0.10213 | 0.23152 | 0.17818 |
| 66 | INOSINE | 0.96229 | -0.055449 | 0.58352 | 0.47758 |
| 67 | JASMONATE | 0.91354 | -0.13046 | 0.07605 | 0.068361 |
| 68 | LAUROYLCARNITINE | 1.0751 | 0.10446 | 0.59277 | 0.9323 |
| 69 | LEUCINE | 1.0143 | 0.020518 | 0.70954 | 0.9774 |
| 70 | Linolenelaidic acid | 0.92886 | -0.10647 | 0.23688 | 0.40951 |
| 71 | LYSINE | 0.98585 | -0.020554 | 0.65952 | 0.62973 |
| 72 | LysoPA(0:0/16:0) | 1.0141 | 0.020167 | 0.6163 | 0.71254 |
| 73 | LysoPC(14:0/0:0) | 0.97359 | -0.038612 | 0.42108 | 0.47758 |
| 74 | LysoPC(16:1/0:0) | 0.9223 | -0.11669 | 0.028541 | 0.044902 |
| 75 | LysoPC(18:0) | 0.97691 | -0.033709 | 0.39526 | 0.37769 |
| 76 | LysoPC(18:1) | 0.97231 | -0.04051 | 0.2369 | 0.15997 |
| 77 | LysoPC(18:2) | 0.98822 | -0.017089 | 0.84412 | 0.9774 |
| 78 | LysoPC(20:4) | 0.99535 | -0.0067297 | 0.89686 | 0.75528 |
| 79 | LysoPC(22:6) | 0.97882 | -0.030887 | 0.62664 | 0.88739 |
| 80 | LysoPE(0:0/20:0) | 1.0397 | 0.056108 | 0.77155 | 0.71254 |
| 81 | LysoPE(0:0/20:1) | 1.0001 | 0.00016657 | 0.99844 | 0.67066 |
| 82 | LysoPE(0:0/22:0) | 1.1243 | 0.16903 | 0.44635 | 0.62973 |
| 83 | LysoPE(0:0/22:2) | 1.0155 | 0.022153 | 0.6712 | 0.62973 |
| 84 | LysoPE(15:0/0:0) | 0.98598 | -0.020373 | 0.76664 | 0.58988 |
| 85 | LysoPE(16:1/0:0) | 0.94404 | -0.083074 | 0.37625 | 0.62973 |
| 86 | LysoPE(18:0/0:0) | 0.93641 | -0.094792 | 0.006593 | 0.006812 |
| 87 | LysoPE(22:6/0:0) | 0.9938 | -0.0089729 | 0.61698 | 0.51372 |
| 88 | LysoPI(18:0/0:0) | 0.96408 | -0.052769 | 0.28798 | 0.34736 |
| 89 | Lysyl-Leucine | 1.0493 | 0.069434 | 0.416 | 0.21892 |
| 90 | Lysyl-Proline | 1.5448 | 0.62738 | 0.13333 | 0.24152 |
| 91 | METHACHOLINE | 0.67197 | -0.57354 | 0.1057 | 0.044902 |
| 92 | Methionine | 1.0893 | 0.12342 | 0.090742 | 0.14317 |
| 93 | Methionine sulfoxide | 0.94363 | -0.083706 | 0.58236 | 0.51372 |
| 94 | Methyl linoleate | 1.1672 | 0.223 | 0.19337 | 0.31859 |
| 95 | Methyladenosine | 0.95107 | -0.072377 | 0.41699 | 0.75528 |
| 96 | 5-Methyldeoxycytidine | 1.0184 | 0.026285 | 0.89121 | 0.62973 |
| 97 | 5'-METHYLTHIOADENOSINE | 1.0079 | 0.011375 | 0.87944 | 0.67066 |
| 98 | MG(0:0/22:6/0:0) | 0.97983 | -0.02939 | 0.52454 | 0.88739 |
| 99 | Myristoylcarnitine | 1.0274 | 0.038979 | 0.73322 | 0.88739 |
| 100 | NICOTINAMIDE | 0.85819 | -0.22063 | 0.041459 | 0.033241 |
| 101 | Octadecanamide | 1.1426 | 0.19229 | 0.60251 | 0.88739 |
| 102 | 9-Octadecenal | 1.0557 | 0.078212 | 0.23255 | 0.37769 |
| 103 | Octadecenoic acid | 0.82716 | -0.27375 | 0.2266 | 0.19781 |
| 104 | Octadecenoylcarnitine | 1.0353 | 0.050037 | 0.59964 | 0.67066 |
| 105 | OCTADECYLPHOSPHOCHOLINE | 1.1943 | 0.25617 | 0.13135 | 0.12769 |
| 106 | Oleamide | 1.0405 | 0.05721 | 0.83381 | 0.75528 |
| 107 | Oleic Acid ethyl ester | 1.1392 | 0.188 | 0.44746 | 0.47758 |
| 108 | Oleoylglycerophosphoinositol | 0.93404 | -0.098451 | 0.032145 | 0.038721 |
| 109 | L-OLEOYL-RAC-GLYCEROL | 0.99692 | -0.0044436 | 0.97029 | 1 |
| 110 | PA(17:0/0:0) | 0.83403 | -0.26182 | 0.76898 | 0.88739 |
| 111 | PA(24:0/21:0) | 1.1543 | 0.20697 | 0.00847 | 0.010045 |
| 112 | Palmitic Acid ethyl ester | 1.0814 | 0.11295 | 0.69301 | 0.67066 |
| 113 | Palmitoyl carnitine | 0.98128 | -0.02726 | 0.79472 | 0.9323 |
| 114 | D-PANTOTHENIC ACID | 0.91841 | -0.12279 | 0.44131 | 0.24152 |
| 115 | PC(16:0/18:2) | 1.0622 | 0.087093 | 0.19367 | 0.31859 |
| 116 | PC(16:0/20:1) | 0.96892 | -0.045558 | 0.43047 | 0.17818 |
| 117 | PC(16:0/22:1) | 0.96967 | -0.044434 | 0.46283 | 0.44283 |
| 118 | PC(18:0/20:4) | 1.0234 | 0.033314 | 0.5877 | 0.37769 |
| 119 | PC(22:0/18:3) | 1.1453 | 0.1957 | 0.095676 | 0.12769 |
| 120 | PC(22:2/20:5) | 1.7295 | 0.79038 | 0.023517 | 0.044902 |
| 121 | PC(22:6/18:2) | 1.0428 | 0.060458 | 0.3108 | 0.62973 |
| 122 | PC(24:1/18:4) | 0.98977 | -0.014835 | 0.75298 | 0.67066 |
| 123 | PE(16:0/0:0) | 0.97305 | -0.039407 | 0.4412 | 0.47758 |
| 124 | PE(16:0/0:0) | 0.88248 | -0.18037 | 0.004711 | 0.002316 |
| 125 | PE(16:0/22:4) | 0.88582 | -0.17491 | 0.46478 | 0.19781 |
| 126 | PE(17:1/0:0) | 0.99374 | -0.0090588 | 0.91071 | 0.62973 |
| 127 | PE(18:0/22:2) | 0.99971 | -0.00041769 | 0.99474 | 0.58988 |
| 128 | PE(19:1/0:0) | 0.93752 | -0.09308 | 0.071402 | 0.1135 |
| 129 | PE(22:2/20:5) | 1.0162 | 0.023228 | 0.59197 | 0.44283 |
| 130 | PE(22:4/15:0) | 0.89586 | -0.15865 | 0.11185 | 0.19781 |
| 131 | PE(22:6/22:6) | 1.025 | 0.035621 | 0.42526 | 0.55117 |
| 132 | PE(24:0/22:4) | 0.99079 | -0.013353 | 0.88939 | 0.62973 |
| 133 | PHENACYLAMINE | 1.1456 | 0.19606 | 0.016769 | 0.038721 |
| 134 | PIPECOLINIC ACID | 1.1458 | 0.19637 | 0.65217 | 0.51372 |
| 135 | Propionylcarnitine | 1.1832 | 0.24267 | 0.24733 | 0.24152 |
| 136 | PS(18:1/0:0) | 1.0216 | 0.030778 | 0.78996 | 0.9323 |
| 137 | PS(18:3/20:0) | 0.95834 | -0.061391 | 0.33472 | 0.21892 |
| 138 | PS(18:3/22:0) | 0.98501 | -0.021796 | 0.67238 | 0.9323 |
| 139 | PS(18:4/22:2) | 1.1563 | 0.20949 | 0.39169 | 0.55117 |
| 140 | PS(20:1/20:0) | 1.0402 | 0.056865 | 0.2969 | 0.19781 |
| 141 | PS(20:4/20:0) | 0.90917 | -0.13737 | 0.015538 | 0.038721 |
| 142 | PS(20:4/22:0) | 0.94405 | -0.083061 | 0.2681 | 0.21892 |
| 143 | SERINE | 1.0323 | 0.04587 | 0.47766 | 0.79875 |
| 144 | Spermic acid | 1.0304 | 0.043233 | 0.76607 | 0.88739 |
| 145 | SPERMIDINE | 1.1474 | 0.19838 | 0.1849 | 0.15997 |
| 146 | Sphinganine | 1.0199 | 0.02838 | 0.41821 | 0.79875 |
| 147 | Succinyladenosine | 0.83647 | -0.25761 | 0.020161 | 0.020489 |
| 148 | TAURINE | 0.93864 | -0.091363 | 0.045387 | 0.051865 |
| 149 | TG(14:1/20:5/22:6) | 0.92692 | -0.10949 | 0.61727 | 0.47758 |
| 150 | TG(18:4/18:3/18:4) | 0.92258 | -0.11626 | 0.17408 | 0.19781 |
| 151 | Trihydroxyvitamin D3 | 0.85124 | -0.23237 | 0.095592 | 0.1135 |
| 152 | NE,NE,NE-TRIMETHYLLYSINE | 0.97134 | -0.041955 | 0.5154 | 0.51372 |
| 153 | Uracil | 1.0442 | 0.062365 | 0.48777 | 0.44283 |
| 154 | Urea | 1.011 | 0.01584 | 0.92937 | 0.038721 |
| 155 | Uric acid | 1.1931 | 0.25469 | 0.3228 | 0.26567 |
| 156 | Uridine | 0.99021 | -0.014189 | 0.80813 | 0.9323 |
| 157 | Valyl-Asparagine | 0.98709 | -0.018745 | 0.71892 | 0.67066 |
| 158 | Vitamin A | 1.156 | 0.20919 | 0.26 | 0.40951 |
| 159 | XANTHINE | 0.93811 | -0.092173 | 0.24133 | 0.26567 |
| 160 | Cer(18:1/18:0) | 1.0541 | 0.075945 | 0.049331 | 0.044902 |
| 161 | Cer(d18:0/18:1) | 1.2039 | 0.26777 | 0.13821 | 0.068361 |
| 162 | Cer(d18:0/18:1)\_iso2 | 1.0258 | 0.036685 | 0.32219 | 0.31859 |
| 163 | Cer(d18:0/20:0) | 1.0841 | 0.11646 | 0.50907 | 0.44283 |
| 164 | Cer(d18:0/22:0) | 1.0319 | 0.04532 | 0.78685 | 0.55117 |
| 165 | Cer(d18:1/16:0)( N-Palmitoylsphingosine) | 1.1258 | 0.17099 | 0.076974 | 0.10053 |
| 166 | Cer(d18:1/18:1) | 1.0464 | 0.06547 | 0.38193 | 0.24152 |
| 167 | Cer(d18:1/18:1)\_iso2 | 1.0678 | 0.094628 | 0.030958 | 0.059657 |
| 168 | Cer(d18:1/20:0) | 1.0198 | 0.028252 | 0.72226 | 0.71254 |
| 169 | Cer(d18:1/22:1) | 0.93679 | -0.094197 | 0.64493 | 0.75528 |
| 170 | Cer(d18:1/24:1) | 0.91419 | -0.12944 | 0.51456 | 0.51372 |
| 171 | Cer(t18:0/16:0) | 1.1551 | 0.20801 | 0.27575 | 0.29134 |
| 172 | Dihydroceramide | 1.0972 | 0.13379 | 0.15536 | 0.059657 |
| 173 | C2-Dihydroceramide | 0.84041 | -0.25084 | 0.5059 | 0.79875 |
| 174 | HexHexCer(d18:1/18:1) | 1.1213 | 0.16523 | 0.43253 | 0.79875 |
| 175 | HexCer(d18:1/16:0) | 0.98749 | -0.018158 | 0.87201 | 0.71254 |
| 176 | HexCer(d18:1/18:1) | 0.9993 | -0.0010062 | 0.98328 | 0.88739 |
| 177 | HexCer(d18:1/20:0) | 0.99488 | -0.0074092 | 0.89068 | 0.88739 |
| 178 | HexCer(d18:1/18:0) | 0.98716 | -0.018649 | 0.58896 | 0.62973 |
| 179 | HexCer(d18:1/24:1) | 1.1906 | 0.25164 | 0.44021 | 0.58988 |
| 180 | HexHexCer(d18:1/18:0) | 1.0328 | 0.046596 | 0.67658 | 0.9323 |

**Table 3. WT1000 versus WT0**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  |  |  | **Parametric test** | **Non-parametric test** |
|  | **Compound** | **Fold Change** | **Fold change (log2)** | **p-value** | **p-value** |
| 1 | Acetylcarnitine | 1.3503 | 0.43325 | 0.15196 | 0.078893 |
| 2 | Acetylcholine | 0.97412 | -0.037823 | 0.63513 | 0.40018 |
| 3 | N-ACETYL-L-ASPARTIC ACID | 0.96022 | -0.058557 | 0.55023 | 0.90483 |
| 4 | N-ACETYLNEURAMINATE | 1.0357 | 0.050643 | 0.50316 | 0.84211 |
| 5 | N1-Acetylspermidine | 1.1995 | 0.26239 | 0.18177 | 0.24281 |
| 6 | ADENINE | 0.91595 | -0.12666 | 0.70046 | 0.54896 |
| 7 | ADENOSINE | 0.91757 | -0.12411 | 0.57533 | 0.90483 |
| 8 | Adrenic acid | 1.1261 | 0.17131 | 0.089249 | 0.11275 |
| 9 | ALANINE | 1.0079 | 0.011416 | 0.88579 | 0.96824 |
| 10 | 4-AMINOBUTANOIC ACID | 1.0191 | 0.027341 | 0.66127 | 0.90483 |
| 11 | L-AMINOCYCLOPROPANE-1-CARBOXYLATE | 1.0171 | 0.024435 | 0.65499 | 0.96824 |
| 12 | 2-AMINOETHYL DIHYDROGEN PHOSPHATE | 1.0679 | 0.094735 | 0.69944 | 0.44697 |
| 13 | 5-AMINOPENTANOATE | 0.91318 | -0.13104 | 0.22145 | 0.27751 |
| 14 | Arachidonic acid ethyl ester | 1.2309 | 0.29966 | 0.28092 | 0.35623 |
| 15 | ARGININE | 0.96272 | -0.054805 | 0.45688 | 0.35623 |
| 16 | Argininosuccinic acid | 0.96303 | -0.054341 | 0.64746 | 0.90483 |
| 17 | AZELAIC ACID | 0.91049 | -0.13528 | 0.28886 | 0.31538 |
| 18 | C16 Sphingosine | 0.88067 | -0.18332 | 0.32643 | 0.35623 |
| 19 | Campesterol | 0.80953 | -0.30484 | 0.35644 | 0.40018 |
| 20 | CARNOSINE | 1.0563 | 0.07896 | 0.59942 | 0.4967 |
| 21 | Cytidine diphosphate choline (CDPcholine) | 0.94559 | -0.080706 | 0.66304 | 0.78019 |
| 22 | Cholesterol | 1.0097 | 0.013949 | 0.74596 | 0.60378 |
| 23 | CITRATE | 0.95229 | -0.070528 | 0.40059 | 0.66072 |
| 24 | CITRULLINE | 1.0094 | 0.013486 | 0.94074 | 0.7197 |
| 25 | CMP | 0.95189 | -0.071126 | 0.55838 | 0.96824 |
| 26 | CREATINE | 1.0145 | 0.020703 | 0.41801 | 0.54896 |
| 27 | CYSTEINE | 1.167 | 0.22284 | 0.31376 | 0.1564 |
| 28 | Cysteineglutathione disulfide | 1.1204 | 0.16399 | 0.45873 | 0.66072 |
| 29 | CYTIDINE | 1.161 | 0.21537 | 0.13333 | 0.27751 |
| 30 | CYTOSINE | 1.0785 | 0.109 | 0.49412 | 0.90483 |
| 31 | D-Aspartic acid | 0.92892 | -0.10638 | 0.31831 | 0.4967 |
| 32 | N-(1-Deoxy-1-fructosyl)alanine | 1.042 | 0.059339 | 0.54479 | 1 |
| 33 | DEOXYCARNITINE | 1.0708 | 0.098714 | 0.34405 | 0.44697 |
| 34 | DESMOSTEROL | 1.0138 | 0.019733 | 0.71548 | 0.66072 |
| 35 | DG(16:0/18:0/0:0) | 1.0282 | 0.040052 | 0.69465 | 0.78019 |
| 36 | DG(20:2/0:0/22:6) | 1.1026 | 0.14089 | 0.07202 | 0.1333 |
| 37 | DG(22:0/0:0/20:4) | 1.7864 | 0.83708 | 0.0072283 | 0.010132 |
| 38 | DG(20:4/24:0/0:0) | 1.5697 | 0.65053 | 0.015866 | 0.022018 |
| 39 | 17,21-DIHYDROXY-4-PREGNENE-3,20-DIONE | 1.3969 | 0.48218 | 0.3681 | 0.40018 |
| 40 | N,N-dimethyl-Safingol | 0.9904 | -0.013922 | 0.93377 | 0.96824 |
| 41 | Docosapentaenoic acid | 1.5752 | 0.65551 | 0.087649 | 0.09472 |
| 42 | Docosatrienoic acid | 0.94536 | -0.081066 | 0.49655 | 0.54896 |
| 43 | Dodecanoic acid | 1.411 | 0.49676 | 0.11905 | 0.1333 |
| 44 | dUMP | 0.98409 | -0.023141 | 0.57738 | 0.60378 |
| 45 | Eicosatrienoic acid | 0.97092 | -0.042575 | 0.62579 | 0.66072 |
| 46 | Ergothioneine | 1.3078 | 0.38717 | 0.014399 | 0.010132 |
| 47 | 4-O-Galactopyranosylxylose | 1.0897 | 0.12389 | 0.28829 | 0.60378 |
| 48 | GLUTAMIC ACID | 1.0405 | 0.057252 | 0.092822 | 0.053476 |
| 49 | L-GLUTAMINE | 1.0636 | 0.088907 | 0.25305 | 0.35623 |
| 50 | gamma-Glutamylglutamic acid | 1.0815 | 0.11302 | 0.40396 | 0.35623 |
| 51 | GLUTATHIONE | 0.99069 | -0.013492 | 0.94248 | 0.7197 |
| 52 | Glycerophosphocholine | 1.0184 | 0.026279 | 0.91924 | 0.7197 |
| 53 | GLYCINE | 0.94164 | -0.086755 | 0.5747 | 0.60378 |
| 54 | GLYCOCHOLATE | 1.1612 | 0.21563 | 0.13273 | 0.21102 |
| 55 | Guanidylic acid (guanosine monophosphate) | 0.95202 | -0.070939 | 0.91746 | 1 |
| 56 | GUANINE | 1.0297 | 0.042255 | 0.71108 | 0.54896 |
| 57 | Guanosine | 1.0303 | 0.043005 | 0.46218 | 0.90483 |
| 58 | 16-HETE | 0.82259 | -0.28175 | 0.58778 | 0.96824 |
| 59 | HISTIDINE | 1.078 | 0.1083 | 0.15566 | 0.1564 |
| 60 | Homoanserine | 1.1394 | 0.18824 | 0.10167 | 0.1564 |
| 61 | 14-Hydroperoxy-H4-neuroprostane | 1.6414 | 0.71495 | 0.32529 | 0.11275 |
| 62 | 12-HYDROXYDODECANOIC ACID | 1.1288 | 0.17477 | 0.043287 | 0.065254 |
| 63 | 5-Hydroxyindoleacetic acid | 0.92324 | -0.11523 | 0.66127 | 1 |
| 64 | 13-hydroxyoctadecanoic acid | 1.1079 | 0.14777 | 0.77669 | 0.90483 |
| 65 | HYPOXANTHINE | 0.95422 | -0.067603 | 0.52558 | 0.40018 |
| 66 | INOSINE | 0.89336 | -0.16269 | 0.094925 | 0.027929 |
| 67 | JASMONATE | 1.1102 | 0.15076 | 0.069209 | 0.053476 |
| 68 | LAUROYLCARNITINE | 1.2311 | 0.29995 | 0.21535 | 0.21102 |
| 69 | LEUCINE | 1.0143 | 0.02044 | 0.82646 | 0.60378 |
| 70 | Linolenelaidic acid | 1.0123 | 0.017591 | 0.88485 | 0.84211 |
| 71 | LYSINE | 1.059 | 0.082649 | 0.41564 | 1 |
| 72 | LysoPA(0:0/16:0) | 0.97669 | -0.034029 | 0.62759 | 0.54896 |
| 73 | LysoPC(14:0/0:0) | 0.97838 | -0.031536 | 0.60372 | 0.4967 |
| 74 | LysoPC(16:1/0:0) | 1.0582 | 0.08158 | 0.26332 | 0.40018 |
| 75 | LysoPC(18:0) | 0.96823 | -0.046573 | 0.51134 | 0.1564 |
| 76 | LysoPC(18:1) | 1.0106 | 0.015218 | 0.8252 | 0.96824 |
| 77 | LysoPC(18:2) | 1.0248 | 0.035361 | 0.78018 | 0.84211 |
| 78 | LysoPC(20:4) | 1.0399 | 0.056469 | 0.6285 | 0.90483 |
| 79 | LysoPC(22:6) | 0.95869 | -0.060868 | 0.59352 | 0.44697 |
| 80 | LysoPE(0:0/20:0) | 0.80345 | -0.31572 | 0.16648 | 0.31538 |
| 81 | LysoPE(0:0/20:1) | 0.98811 | -0.017254 | 0.86522 | 0.96824 |
| 82 | LysoPE(0:0/22:0) | 0.90121 | -0.15007 | 0.54037 | 0.4967 |
| 83 | LysoPE(0:0/22:2) | 1.1062 | 0.14559 | 0.0085082 | 0.010132 |
| 84 | LysoPE(15:0/0:0) | 0.88501 | -0.17623 | 0.32633 | 0.66072 |
| 85 | LysoPE(16:1/0:0) | 0.9916 | -0.012173 | 0.91372 | 0.78019 |
| 86 | LysoPE(18:0/0:0) | 1.0283 | 0.040285 | 0.58634 | 1 |
| 87 | LysoPE(22:6/0:0) | 1.0024 | 0.0034954 | 0.90971 | 0.78019 |
| 88 | LysoPI(18:0/0:0) | 0.95137 | -0.071915 | 0.38897 | 0.66072 |
| 89 | Lysyl-Leucine | 1.3468 | 0.42954 | 0.015883 | 0.027929 |
| 90 | Lysyl-Proline | 1.0933 | 0.12866 | 0.75116 | 0.96824 |
| 91 | METHACHOLINE | 0.84198 | -0.24814 | 0.64094 | 0.7197 |
| 92 | Methionine | 1.0239 | 0.034082 | 0.75623 | 0.4967 |
| 93 | Methionine sulfoxide | 0.99707 | -0.0042404 | 0.97995 | 0.96824 |
| 94 | Methyl linoleate | 1.1528 | 0.20509 | 0.35411 | 0.40018 |
| 95 | Methyladenosine | 0.93523 | -0.09661 | 0.40989 | 0.40018 |
| 96 | 5-Methyldeoxycytidine | 1.3886 | 0.47364 | 0.019623 | 0.027929 |
| 97 | 5'-METHYLTHIOADENOSINE | 0.82056 | -0.28532 | 0.045718 | 0.022018 |
| 98 | MG(0:0/22:6/0:0) | 0.97033 | -0.043451 | 0.50223 | 0.27751 |
| 99 | Myristoylcarnitine | 1.1442 | 0.19435 | 0.15634 | 0.40018 |
| 100 | NICOTINAMIDE | 1.0462 | 0.065217 | 0.59157 | 0.60378 |
| 101 | Octadecanamide | 1.0145 | 0.020802 | 0.92376 | 0.78019 |
| 102 | 9-Octadecenal | 0.9689 | -0.045585 | 0.44756 | 0.31538 |
| 103 | Octadecenoic acid | 1.3992 | 0.48464 | 0.060112 | 0.18232 |
| 104 | Octadecenoylcarnitine | 1.1501 | 0.20179 | 0.13464 | 0.35623 |
| 105 | OCTADECYLPHOSPHOCHOLINE | 1.0748 | 0.10406 | 0.50049 | 1 |
| 106 | Oleamide | 0.88439 | -0.17724 | 0.50879 | 0.4967 |
| 107 | Oleic Acid ethyl ester | 1.2789 | 0.35488 | 0.30489 | 0.31538 |
| 108 | Oleoylglycerophosphoinositol | 1.0035 | 0.0050469 | 0.94601 | 0.7197 |
| 109 | L-OLEOYL-RAC-GLYCEROL | 1.1162 | 0.15854 | 0.20104 | 0.27751 |
| 110 | PA(17:0/0:0) | 0.67902 | -0.55847 | 0.60838 | 0.90483 |
| 111 | PA(24:0/21:0) | 0.99653 | -0.0050162 | 0.9618 | 0.78019 |
| 112 | Palmitic Acid ethyl ester | 1.2381 | 0.30814 | 0.32223 | 0.35623 |
| 113 | Palmitoyl carnitine | 1.0268 | 0.038153 | 0.81734 | 0.90483 |
| 114 | D-PANTOTHENIC ACID | 0.94118 | -0.087458 | 0.69525 | 0.1333 |
| 115 | PC(16:0/18:2) | 1.0556 | 0.078005 | 0.33434 | 0.35623 |
| 116 | PC(16:0/20:1) | 0.92889 | -0.10642 | 0.23991 | 0.60378 |
| 117 | PC(16:0/22:1) | 0.92383 | -0.1143 | 0.16737 | 0.40018 |
| 118 | PC(18:0/20:4) | 1.0889 | 0.12286 | 0.23769 | 0.18232 |
| 119 | PC(22:0/18:3) | 0.93007 | -0.10459 | 0.49325 | 0.54896 |
| 120 | PC(22:2/20:5) | 1.4154 | 0.50125 | 0.12234 | 0.09472 |
| 121 | PC(22:6/18:2) | 1.0314 | 0.044593 | 0.42929 | 0.35623 |
| 122 | PC(24:1/18:4) | 1.0796 | 0.11054 | 0.41416 | 0.44697 |
| 123 | PE(16:0/0:0) | 1.0298 | 0.042416 | 0.56602 | 0.84211 |
| 124 | PE(16:0/0:0) | 1.0385 | 0.054455 | 0.54953 | 0.84211 |
| 125 | PE(16:0/22:4) | 1.0812 | 0.11259 | 0.46936 | 0.54896 |
| 126 | PE(17:1/0:0) | 1.053 | 0.074469 | 0.48691 | 0.44697 |
| 127 | PE(18:0/22:2) | 1.0634 | 0.08873 | 0.17876 | 0.21102 |
| 128 | PE(19:1/0:0) | 1.0795 | 0.11042 | 0.29596 | 0.44697 |
| 129 | PE(22:2/20:5) | 1.0994 | 0.13674 | 0.02065 | 0.027929 |
| 130 | PE(22:4/15:0) | 1.0296 | 0.042092 | 0.72309 | 0.4967 |
| 131 | PE(22:6/22:6) | 1.0683 | 0.095359 | 0.13488 | 0.1564 |
| 132 | PE(24:0/22:4) | 0.87487 | -0.19285 | 0.14014 | 0.11275 |
| 133 | PHENACYLAMINE | 1.0843 | 0.11671 | 0.33105 | 0.66072 |
| 134 | PIPECOLINIC ACID | 1.0259 | 0.036937 | 0.92044 | 0.78019 |
| 135 | Propionylcarnitine | 1.0862 | 0.11934 | 0.67637 | 1 |
| 136 | PS(18:1/0:0) | 1.2605 | 0.33398 | 0.037621 | 0.017212 |
| 137 | PS(18:3/20:0) | 1.0472 | 0.066534 | 0.568 | 0.78019 |
| 138 | PS(18:3/22:0) | 1.0503 | 0.070787 | 0.29445 | 0.4967 |
| 139 | PS(18:4/22:2) | 1.2441 | 0.31507 | 0.22709 | 0.40018 |
| 140 | PS(20:1/20:0) | 0.9843 | -0.022829 | 0.70538 | 0.4967 |
| 141 | PS(20:4/20:0) | 0.97774 | -0.032484 | 0.7119 | 0.54896 |
| 142 | PS(20:4/22:0) | 1.0726 | 0.10111 | 0.43457 | 0.31538 |
| 143 | SERINE | 1.0449 | 0.063335 | 0.60836 | 0.96824 |
| 144 | Spermic acid | 1.2557 | 0.32855 | 0.064391 | 0.078893 |
| 145 | SPERMIDINE | 1.2746 | 0.35001 | 0.15265 | 0.18232 |
| 146 | Sphinganine | 1.0379 | 0.053679 | 0.28965 | 0.4967 |
| 147 | Succinyladenosine | 0.86878 | -0.20294 | 0.14021 | 0.1564 |
| 148 | TAURINE | 1.0309 | 0.043896 | 0.54894 | 0.84211 |
| 149 | TG(14:1/20:5/22:6) | 1.0189 | 0.026969 | 0.91297 | 0.66072 |
| 150 | TG(18:4/18:3/18:4) | 0.94442 | -0.082504 | 0.57259 | 0.60378 |
| 151 | Trihydroxyvitamin D3 | 1.2613 | 0.33493 | 0.023805 | 0.043474 |
| 152 | NE,NE,NE-TRIMETHYLLYSINE | 0.96952 | -0.044654 | 0.63026 | 0.44697 |
| 153 | Uracil | 1.1014 | 0.13938 | 0.14589 | 0.31538 |
| 154 | Urea | 1.1546 | 0.20741 | 0.0057209 | 0.010132 |
| 155 | Uric acid | 1.1459 | 0.19653 | 0.72809 | 0.66072 |
| 156 | Uridine | 0.95221 | -0.07065 | 0.42979 | 0.54896 |
| 157 | Valyl-Asparagine | 1.061 | 0.085399 | 0.60254 | 0.96824 |
| 158 | Vitamin A | 1.2776 | 0.35338 | 0.16558 | 0.27751 |
| 159 | XANTHINE | 0.99082 | -0.013301 | 0.9196 | 0.60378 |
| 160 | Cer(18:1/18:0) | 0.99019 | -0.014218 | 0.86701 | 0.7197 |
| 161 | Cer(d18:0/18:1) | 1.0126 | 0.018031 | 0.93133 | 0.84211 |
| 162 | Cer(d18:0/18:1)\_iso2 | 1.0348 | 0.049341 | 0.43461 | 0.66072 |
| 163 | Cer(d18:0/20:0) | 0.99845 | -0.0022315 | 0.99121 | 0.84211 |
| 164 | Cer(d18:0/22:0) | 0.77147 | -0.37432 | 0.091126 | 0.11275 |
| 165 | Cer(d18:1/16:0)( N-Palmitoylsphingosine) | 1.2043 | 0.26819 | 0.1066 | 0.21102 |
| 166 | Cer(d18:1/18:1) | 1.0754 | 0.10493 | 0.15032 | 0.40018 |
| 167 | Cer(d18:1/18:1)\_iso2 | 1.0863 | 0.11948 | 0.15872 | 0.44697 |
| 168 | Cer(d18:1/20:0) | 1.0067 | 0.0096389 | 0.93159 | 0.96824 |
| 169 | Cer(d18:1/22:1) | 0.66161 | -0.59595 | 0.055362 | 0.1333 |
| 170 | Cer(d18:1/24:1) | 0.98275 | -0.025097 | 0.93629 | 1 |
| 171 | Cer(t18:0/16:0) | 1.2583 | 0.3315 | 0.14595 | 0.1564 |
| 172 | Dihydroceramide | 1.064 | 0.089479 | 0.081716 | 0.065254 |
| 173 | C2-Dihydroceramide | 1.1157 | 0.15791 | 0.36533 | 0.27751 |
| 174 | HexHexCer(d18:1/18:1) | 1.2671 | 0.34157 | 0.038601 | 0.034987 |
| 175 | HexCer(d18:1/16:0) | 1.0424 | 0.059897 | 0.5219 | 0.96824 |
| 176 | HexCer(d18:1/18:1) | 1.0278 | 0.039603 | 0.6865 | 0.60378 |
| 177 | HexCer(d18:1/20:0) | 1.0723 | 0.10064 | 0.17849 | 0.44697 |
| 178 | HexCer(d18:1/18:0) | 0.99358 | -0.0092873 | 0.87072 | 0.84211 |
| 179 | HexCer(d18:1/24:1) | 0.91791 | -0.12358 | 0.79514 | 0.78019 |
| 180 | HexHexCer(d18:1/18:0) | 1.1205 | 0.16419 | 0.10265 | 0.18232 |