

Supplementary Materials

Table S1. A total of 183 metabolites were identified and their concentrations were determined.

| RT | Peaks | VIP | p value | FC(T/O) | VIP | p value | FC(T/N) | VIP | p value | FC(O/N) |
|---------|-------------------------------------|----------|------------|--------------|-----------|-------------|----------|---------|----------|----------|
| 11.2204 | Citraconic acid degr1 | 0.009634 | 0.98350859 | 1.087158482 | 0.994365 | 0.018730906 | 1.413805 | 1.30659 | 0.000283 | 1.300459 |
| 9.29662 | 4-Androsten-11beta-ol-3,17-dione 1 | 1.29E-01 | 0.78055717 | 1.055616439 | 0.865751 | 0.040977594 | 7.04258 | 1.19957 | 0.001032 | 6.671533 |
| 25.8678 | malonic acid 1 | 1.32E-01 | 0.78096838 | 0.880294483 | 0.778666 | 0.054565967 | 0.602697 | 1.00238 | 0.009441 | 0.684654 |
| 26.9555 | L-Threose 1 | 0.204483 | 0.6592374 | 1.314593964 | 0.921838 | 0.016945786 | 0.487327 | 1.01342 | 0.011871 | 0.370706 |
| 10.9712 | proline | 0.307567 | 0.52229702 | 1.538691623 | 0.590557 | 0.180285553 | 6.267738 | 1.01306 | 0.006378 | 4.07342 |
| 20.4153 | galactose 2 | 0.415009 | 0.3714367 | 1.532244605 | 0.774153 | 0.046661072 | 0.557011 | 1.08732 | 0.004593 | 0.363526 |
| 11.7222 | Pelargonic acid | 0.476293 | 0.2791267 | 0.694617469 | 0.718819 | 0.103854977 | 3.208783 | 1.04436 | 0.010129 | 4.619497 |
| 8.11328 | lactic acid | 0.538541 | 0.22637481 | 0.630658 | 0.546646 | 0.219305262 | 154.9214 | 1.11532 | 0.005682 | 245.6504 |
| 16.0173 | fucose 2 | 0.654089 | 0.12957195 | 0.615286565 | 0.847032 | 0.045937828 | 6.091312 | 1.18565 | 0.00219 | 9.899959 |
| 13.4598 | indole-3-acetic acid | 0.662111 | 0.16907266 | 21801.11708 | 0.800574 | 0.043375103 | 0.709929 | 1.35587 | 0.000422 | 3.26E-05 |
| 24.8044 | malonic acid 1 | 0.701519 | 0.13607262 | 1.655901343 | 0.696055 | 0.08046902 | 0.6138 | 1.23594 | 0.001184 | 0.370675 |
| 25.6064 | Linoleic acid methyl ester | 7.92E-01 | 0.0858572 | 1.521247031 | 0.495741 | 2.50E-01 | 0.894917 | 1.41231 | 9.62E-06 | 0.588279 |
| 13.7621 | Glucose-1-phosphate | 0.817509 | 0.06157299 | 0.8804508 | 0.45079 | 0.2766363 | 1.249178 | 1.13931 | 0.0015 | 1.418794 |
| 29.0115 | beta-Mannosylglycerate 2 | 0.893748 | 0.05310125 | 0.7873863880 | 0.467242 | 9.16E-01 | 1.15773 | 1.43988 | 1.03E-05 | 1.470345 |
| 14.0543 | oxoproline | 0.95519 | 0.03433365 | 1.379915679 | 0.210184 | 0.626676416 | 1.140831 | 1.05718 | 0.004065 | 0.826739 |
| 25.657 | linolenic acid | 1.02162 | 0.02842037 | 3.522414474 | 0.323145 | 4.65E-01 | 1.267257 | 1.4548 | 2.96E-06 | 0.359769 |
| 10.3809 | 2-Deoxyerythritol | 1.13569 | 0.01508373 | 242719.2238 | 0.340496 | 0.4207809 | 1.690894 | 1.06368 | 0.008759 | 6.97E-06 |
| 20.5299 | D-erythronolactone 2 | 1.14802 | 0.00507242 | 2.371431828 | 0.590181 | 0.135883604 | 0.627303 | 1.20018 | 0.001171 | 0.264525 |
| 24.6748 | Indolelactate 2 | 1.18107 | 0.00607364 | 0.52003833 | 0.112128 | 0.792147985 | 2.278772 | 1.31899 | 0.00011 | 4.381931 |
| 32.1968 | 2-Monoolein | 1.18636 | 0.00373925 | 0.649446067 | 0.786958 | 0.0417748 | 1.594694 | 1.2867 | 0.000441 | 2.455468 |
| 20.0337 | 2-Keto-L-gulonic acid | 1.19302 | 0.00811016 | 0.372323929 | 0.900726 | 3.96E-02 | 82152.04 | 1.69295 | 2.78E-09 | 220646.7 |
| 20.1654 | glucose 2 | 1.20407 | 0.00207157 | 0.737475691 | 0.580235 | 1.48E-01 | 1.368126 | 1.31256 | 9.55E-05 | 1.855148 |
| 24.9551 | heptadecanoic acid | 1.27584 | 0.00189096 | 1.530331624 | 0.281354 | 0.508718817 | 1.095363 | 1.2535 | 0.000275 | 0.715768 |
| 15.6393 | maleic acid | 1.40E+00 | 0.00011932 | 0.575432763 | 0.511359 | 2.00E-01 | 1.283651 | 1.35612 | 4.14E-05 | 2.230758 |
| 18.9218 | Diglycerol 2 | 1.41E+00 | 0.0007717 | 5.579878683 | 0.549957 | 0.183134585 | 1.340554 | 1.21664 | 0.000966 | 0.240248 |
| 17.4775 | D-(glycerol 1-phosphate) | 1.45708 | 0.00040019 | 6.7716312930 | 0.0645718 | 8.83E-01 | 1.115356 | 1.6113 | 1.72E-09 | 0.16471 |
| 12.2533 | Carnitine | 1.46E+00 | 0.00018935 | 2.5630776980 | 0.0314203 | 0.938987625 | 0.989158 | 1.2655 | 0.000579 | 0.385926 |
| 20.3322 | beta-Mannosylglycerate 1 | 1.47199 | 0.00043945 | 13.64662868 | 0.635223 | 0.106510042 | 0.597729 | 1.29399 | 0.000821 | 0.0438 |
| 27.7594 | Linoleic acid methyl ester | 1.51113 | 8.00E-05 | 1.979801503 | 0.872945 | 3.14E-02 | 1.294023 | 1.3144 | 9.20E-05 | 0.653612 |
| 12.5133 | lactic acid | 1.5124 | 0.00039106 | 3.508823166 | 0.5294 | 0.191664537 | 1.336647 | 1.18808 | 0.002691 | 0.380939 |
| 27.4989 | Zymosterol 2 | 1.52967 | 0.00017414 | 6.789757947 | 0.135171 | 7.47E-01 | 0.991559 | 1.44252 | 4.02E-05 | 0.146037 |
| 12.2537 | Diglycerol 2 | 1.56E+00 | 6.92E-05 | 0.1165833090 | 0.0366401 | 9.32E-01 | 0.997544 | 1.57963 | 5.41E-08 | 8.556488 |
| 25.4705 | Dehydroepiandrosterone | 1.57938 | 0.00016255 | 104301.1186 | 0.305869 | 4.59E-01 | 0.901538 | 1.52555 | 1.99E-05 | 8.64E-06 |
| 9.98655 | Prostaglandin E2 2 | 1.58608 | 3.05E-06 | 4.414348121 | 0.332291 | 0.409270396 | 1.048561 | 1.20494 | 0.001107 | 0.237535 |
| 12.1551 | Ethyl cinnamate | 1.6154 | 8.42E-05 | 167535.3391 | 0.797904 | 0.043193637 | 1.821117 | 1.33917 | 0.000528 | 1.09E-05 |
| 10.6488 | 2-Deoxyerythritol | 1.61633 | 3.50E-05 | 3.970516012 | 0.701324 | 1.01E-01 | 1.245116 | 1.62735 | 7.88E-10 | 0.313591 |
| 20.7883 | fructose 1 | 1.66178 | 3.53E-07 | 17.45153723 | 0.474837 | 0.233190873 | 0.685864 | 1.09007 | 0.006633 | 0.039301 |
| 31.9669 | prunin degr. Prod. 2 | 1.66571 | 2.39E-06 | 2.904023019 | 0.805498 | 4.76E-02 | 1.326741 | 1.56702 | 4.64E-08 | 0.456863 |
| 15.2173 | (+)-Dihydrocarveol | 1.66615 | 2.72E-05 | 105338.1499 | 0.551447 | 1.86E-01 | 0.889834 | 1.66557 | 5.82E-08 | 8.45E-06 |
| 24.4579 | thymidine 5'-monophosphate 1 | 1.67394 | 1.90E-05 | 5.712345652 | 0.986922 | 1.72E-02 | 1.432596 | 1.65926 | 1.54E-08 | 0.250789 |
| 14.2641 | Threonic acid | 1.68E+00 | 1.42E-06 | 0.301079962 | 0.726992 | 6.80E-02 | 0.864943 | 1.57087 | 2.98E-06 | 2.872803 |
| 9.50779 | epsilon-Caprolactam | 1.69549 | 1.48E-08 | 0.127815032 | 0.684604 | 8.05E-02 | 0.441595 | 1.44934 | 3.85E-06 | 3.454957 |
| 20.5483 | methyl heptadecanoate | 1.72874 | 3.13E-06 | 8.728164315 | 0.51846 | 1.97E-01 | 1.233216 | 1.52346 | 1.89E-05 | 0.141292 |
| 23.74 | pentadecanoic acid | 1.74E+00 | 3.50E-07 | 2.834128132 | 0.181295 | 6.63E-01 | 1.082514 | 1.63717 | 4.12E-08 | 0.381957 |
| 25.8734 | N-Methyl-L-glutamic acid 3 | 1.75403 | 1.52E-10 | 12.82253435 | 0.824542 | 3.34E-02 | 1.353106 | 1.60929 | 1.76E-09 | 0.105526 |
| 24.6943 | linolenic acid | 1.75496 | 9.40E-08 | 3.680046879 | 0.953513 | 2.30E-02 | 1.225145 | 1.6928 | 1.39E-14 | 0.332916 |
| 18.4685 | citric acid | 1.79807 | 1.69E-13 | 0.181611602 | 1.28595 | 0.000454624 | 0.278545 | 1.10255 | 0.00472 | 1.53374 |
| 13.393 | cis-1,2-Dihydronaphthalene-1,2-diol | 1.78826 | 1.10E-07 | 131334.5835 | 1.65002 | 1.10E-07 | 205263.7 | 1.51437 | 1.28E-05 | 1.562907 |
| 24.6155 | linoleic acid | 1.77608 | 9.19E-08 | 4.875438327 | 1.46955 | 9.50E-05 | 1.625859 | 1.70565 | 5.17E-16 | 0.333479 |
| 8.53839 | 5-Dihydrocortisol 1 | 1.74736 | 1.66E-06 | 725390.8924 | 1.46128 | 1.21E-05 | 3.131242 | 1.52233 | 2.15E-05 | 4.32E-06 |
| 27.2841 | Analyte 368 | 1.74E+00 | 2.87E-06 | 227592.5879 | 1.01777 | 6.45E-03 | 0.774082 | 1.66915 | 4.31E-08 | 3.4E-06 |
| 27.0315 | stearic acid | 1.72E+00 | 1.62E-07 | 19.04090152 | 1.01293 | 7.54E-03 | 1.496156 | 1.55546 | 2.64E-07 | 0.078576 |

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|---------|---|----------|------------|-------------|---------|-------------|----------|---------|----------|----------|
| 13.3327 | L-Malic acid | 1.71965 | 8.33E-09 | 0.318978532 | 1.48047 | 2.22E-06 | 0.533612 | 1.48351 | 8.33E-06 | 1.672878 |
| 22.3688 | palmitic acid | 1.72E+00 | 3.77E-07 | 2.597038934 | 1.21403 | 3.14E-03 | 1.310076 | 1.66189 | 1.10E-09 | 0.50445 |
| 8.58041 | sarcosine | 1.67E+00 | 1.05E-05 | 2.758681781 | 1.58845 | 3.00E-06 | 3.912536 | 1.42373 | 9.76E-06 | 1.418263 |
| 10.9508 | oxalic acid | 1.66438 | 2.42E-07 | 0.45406346 | 1.30941 | 9.02E-05 | 0.683817 | 1.35653 | 7.05E-05 | 1.505995 |
| 35.3087 | Galactinol 1 | 1.65E+00 | 9.56E-07 | 2.645100348 | 1.23755 | 7.50E-04 | 0.526298 | 1.51435 | 1.63E-05 | 0.198971 |
| 34.5937 | Galactinol 1 | 1.64E+00 | 1.69E-05 | 3.21014742 | 1.30796 | 1.07E-03 | 1.777171 | 1.55192 | 1.56E-07 | 0.553611 |
| 9.66629 | Biphenyl | 1.62405 | 3.66E-06 | 17.9651676 | 1.18834 | 0.00103185 | 2.352245 | 1.17413 | 0.001064 | 0.130934 |
| 9.24869 | 4-aminobutyric acid 3 | 1.60911 | 3.15E-05 | 2.131703821 | 1.56024 | 2.75E-06 | 3.115348 | 1.31506 | 8.95E-05 | 1.461435 |
| 14.0999 | 4-aminobutyric acid 1 | 1.58844 | 4.63E-05 | 2.096403378 | 1.53109 | 5.27E-06 | 2.796614 | 1.10455 | 0.002357 | 1.334006 |
| 24.363 | Turanose 2 | 1.57124 | 1.01E-05 | 0.137923744 | 1.52362 | 1.85E-07 | 0.077869 | 1.27391 | 0.000492 | 0.56458 |
| 21.9989 | fucose 1 | 1.523 | 9.50E-06 | 2.663075242 | 1.26757 | 1.99E-04 | 0.740847 | 1.5856 | 8.64E-09 | 0.278192 |
| 18.237 | shikimic acid | 1.50E+00 | 3.14E-05 | 2.215977415 | 1.56555 | 1.60E-06 | 3.618776 | 1.13777 | 0.002389 | 1.633038 |
| 30.9179 | Tagatose 2 | 1.50E+00 | 7.97E-05 | 0.560972818 | 1.47128 | 2.63E-05 | 0.248739 | 1.35553 | 0.000223 | 0.443407 |
| 24.1337 | 2-Monoolein | 1.50E+00 | 0.00032242 | 3.159254094 | 1.00759 | 0.010305252 | 1.682628 | 1.09282 | 0.004162 | 0.532603 |
| 31.8928 | squalene | 1.49255 | 0.00057821 | 10.05251154 | 1.07845 | 3.05E-03 | 0.5211 | 1.53397 | 1.60E-05 | 0.051838 |
| 14.9356 | Threonic acid | 1.46623 | 0.00015163 | 1.691573375 | 1.55373 | 7.26E-06 | 2.622768 | 1.37532 | 9.06E-05 | 1.55049 |
| 22.7341 | malonic acid 1 | 1.47E+00 | 0.00024607 | 2.152124282 | 1.57874 | 2.64E-06 | 9.649693 | 1.56959 | 1.46E-07 | 4.483799 |
| 14.6339 | 2-Deoxyerythritol | 1.39512 | 0.00013773 | 0.654897436 | 1.48261 | 9.17E-07 | 0.518892 | 1.0082 | 0.006826 | 0.792326 |
| 18.6615 | citrulline 1 | 1.36468 | 0.00098623 | 2.106087356 | 1.52451 | 2.66E-05 | 9.594272 | 1.48913 | 1.08E-05 | 4.555496 |
| 21.882 | myo-inositol | 1.32725 | 0.0013205 | 3.04559E-05 | 1.64595 | 1.62E-08 | 1.61E-05 | 1.13158 | 0.002782 | 0.530231 |
| 21.6943 | oxalic acid | 1.29E+00 | 0.00074413 | 1.579672673 | 1.41891 | 9.15E-06 | 0.564402 | 1.57942 | 8.05E-08 | 0.357291 |
| 11.4168 | uracil | 1.25E+00 | 0.00138283 | 1.750881131 | 1.61431 | 1.45E-07 | 4.280638 | 1.09461 | 0.005904 | 2.444848 |
| 28.3075 | arbutin | 1.22596 | 0.0023782 | 2.475960772 | 1.65816 | 2.74E-08 | 112.401 | 1.07934 | 0.00765 | 45.39691 |
| 23.2809 | trans-3,5-Dimethoxy-4-hydroxycinnamaldehyde 1 | 1.18853 | 0.00261129 | 0.209559478 | 1.48015 | 8.23E-07 | 0.108666 | 1.20292 | 0.000617 | 0.518547 |
| 15.5195 | conduritol b epoxide 2 | 1.13E+00 | 0.005502 | 0.476758422 | 1.4699 | 1.58E-06 | 0.2457 | 1.27139 | 0.000207 | 0.515355 |
| 10.494 | phosphate | 1.10564 | 0.00763385 | 0.678855772 | 1.44491 | 9.42E-06 | 0.319288 | 1.37791 | 0.000139 | 0.470332 |
| 16.6482 | fucose 2 | 1.021 | 0.02398518 | 1.853870876 | 1.25632 | 0.002184839 | 3.285345 | 1.18295 | 0.001624 | 1.772154 |
| 20.1533 | D-Talose 2 | 0.988628 | 0.01602409 | 2.696553201 | 1.25489 | 1.39E-03 | 0.658321 | 1.47514 | 2.70E-05 | 0.244134 |
| 36.681 | 3-Hydroxypropionic acid 1 | 0.983929 | 0.01789453 | 0.536877901 | 1.42088 | 8.67E-06 | 5.442066 | 1.42362 | 5.26E-05 | 10.13651 |
| 11.9122 | L-Allothreonine 1 | 0.982936 | 0.02395272 | 1.356958411 | 1.40088 | 0.000103116 | 1.818817 | 1.28967 | 0.000174 | 1.340363 |
| 9.28022 | N-epsilon-Acetyl-L-lysine 2 | 9.76E-01 | 0.02101741 | 1.30899316 | 1.39429 | 1.36E-05 | 2.135653 | 1.20697 | 0.000642 | 1.631523 |
| 28.6107 | Glucose-1-phosphate | 9.52E-01 | 0.02299942 | 0.862880121 | 1.43509 | 8.27E-06 | 0.540442 | 1.34435 | 0.000132 | 0.626323 |
| 9.58847 | oxalic acid | 9.52E-01 | 0.04392273 | 1.79929318 | 1.00808 | 0.019643776 | 2.118022 | 1.10244 | 0.002933 | 1.177141 |
| 14.5891 | 3,6-Anhydro-D-galactose 1 | 9.31E-01 | 0.02478353 | 0.635100652 | 1.45938 | 1.96E-05 | 0.219908 | 1.42966 | 6.02E-05 | 0.346258 |
| 30.4995 | xylitol | 0.91745 | 0.03441317 | 1.526351169 | 1.63805 | 3.53E-10 | 0.404096 | 1.69488 | 5.51E-15 | 0.264747 |
| 9.41394 | Methyl Phosphate | 0.875393 | 0.05281379 | 1.734781391 | 1.10281 | 2.26E-03 | 0.59537 | 1.41634 | 6.51E-05 | 0.343196 |
| 13.9039 | lactic acid | 8.53E-01 | 0.05583239 | 1.710877431 | 1.4312 | 2.57E-04 | 11155.62 | 1.47729 | 5.75E-05 | 6520.408 |
| 14.3411 | 1-Hydroxyanthraquinone 1 | 8.26E-01 | 0.0671368 | 1.332422068 | 1.19042 | 0.003501694 | 1.732971 | 1.03615 | 0.006514 | 1.300617 |
| 19.9514 | hexadecane | 0.781016 | 0.06458696 | 1.459208663 | 1.62956 | 5.92E-07 | 329446.3 | 1.41327 | 0.00018 | 225770.5 |
| 19.629 | Gluconic lactone 1 | 7.66E-01 | 0.07394879 | 0.799432484 | 1.54458 | 2.22E-05 | 227967.8 | 1.61496 | 1.13E-06 | 285162.1 |
| 10.0679 | Methylmalonic acid | 7.51E-01 | 0.08125995 | 1.446442472 | 1.3954 | 0.000161097 | 2.488917 | 1.10351 | 0.004208 | 1.720717 |
| 21.3247 | isocitric acid 2 | 7.51E-01 | 0.10400487 | 1.241753117 | 1.36637 | 3.81E-05 | 0.426548 | 1.50918 | 1.63E-05 | 0.343505 |
| 15.7238 | Tagatose 1 | 0.751123 | 0.08320387 | 1.22060949 | 1.39324 | 1.64E-05 | 0.669563 | 1.53656 | 1.25E-07 | 0.548548 |
| 17.6124 | Glucose-1-phosphate | 0.749233 | 0.08725167 | 0.888906913 | 1.22118 | 0.001001911 | 0.436916 | 1.17594 | 0.002757 | 0.491521 |
| 13.4967 | glutamine 1 | 0.746189 | 0.09909768 | 1.285210835 | 1.17727 | 0.004457937 | 1.576948 | 1.06127 | 0.006252 | 1.226995 |
| 19.5767 | mannose 1 | 7.29E-01 | 0.09000584 | 0.677389616 | 1.47696 | 1.67E-06 | 11.02811 | 1.24772 | 0.001035 | 16.2803 |
| 17.1768 | fucose 1 | 0.700964 | 0.14361431 | 1.801879715 | 1.02076 | 0.015125149 | 5.814729 | 1.31395 | 0.000326 | 3.227035 |
| 13.81 | aspartic acid 1 | 0.698654 | 0.1235802 | 1.205953604 | 1.51195 | 4.17E-06 | 2.255584 | 1.57683 | 1.56E-08 | 1.870374 |
| 26.8392 | Thioctamide 1 | 0.66648 | 0.12427985 | 0.742552821 | 1.20001 | 0.000753648 | 0.389828 | 1.02714 | 0.006915 | 0.524984 |
| 26.3377 | Carbobenzyloxy-L-leucine degr5 | 6.60E-01 | 0.17076907 | 9870.26941 | 1.31087 | 0.000194113 | 0.170184 | 1.43196 | 0.000132 | 1.72E-05 |
| 11.405 | Glucose-1-phosphate | 0.622598 | 0.16656395 | 0.78467194 | 1.39786 | 3.44E-05 | 0.371582 | 1.39407 | 1.53E-05 | 0.473551 |
| 8.95592 | noradrenaline | 0.617993 | 0.17516187 | 1.224316157 | 1.32024 | 7.43E-04 | 1.711376 | 1.37562 | 6.95E-05 | 1.397822 |
| 20.7827 | Gluconic lactone 2 | 0.593318 | 0.191025 | 0.833955802 | 1.5779 | 1.86E-08 | 0.186015 | 1.61082 | 1.85E-07 | 0.223051 |
| 25.3431 | xylitol | 0.52807 | 0.23021347 | 0.950315412 | 1.37745 | 2.42E-05 | 0.627072 | 1.30976 | 0.000147 | 0.659857 |
| 32.5881 | Lactobionic Acid 1 | 0.490749 | 0.2555066 | 0.296613654 | 1.48243 | 3.49E-06 | 0.067327 | 1.29686 | 0.000129 | 0.226986 |
| 11.0096 | 2-Monoolein | 0.464653 | 0.31851181 | 0.877573408 | 1.35564 | 3.30E-05 | 0.348462 | 1.40076 | 8.27E-05 | 0.397075 |
| 10.815 | 1,5-Anhydroglucitol | 0.463336 | 0.31496021 | 2.265148922 | 1.51931 | 5.53E-07 | 0.145041 | 1.63427 | 4.91E-10 | 0.064032 |
| 13.7325 | malonic acid 2 | 0.458553 | 0.33269008 | 1.297526238 | 1.15247 | 0.001221994 | 0.429651 | 1.35981 | 0.00028 | 0.331131 |
| 20.0802 | glucose 2 | 0.429684 | 0.32023532 | 0.011271375 | 1.51446 | 1.02E-05 | 0.002242 | 1.12665 | 0.002305 | 0.198869 |
| 21.8105 | isocitric acid 2 | 4.22E-01 | 0.37064676 | 1.200024241 | 1.12732 | 0.002004836 | 0.396265 | 1.28361 | 0.000856 | 0.330214 |
| 26.6474 | Galactinol 3 | 4.11E-01 | 0.35893683 | 1.73172267 | 1.00054 | 0.008528398 | 0.278932 | 1.12712 | 0.003685 | 0.161072 |
| 15.283 | 2-Monoolein | 4.08E-01 | 0.36840831 | 0.569415354 | 1.35761 | 3.30E-05 | 0.177292 | 1.36264 | 4.83E-05 | 0.311357 |

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|----------|--|----------|------------|-------------|---------|-------------|----------|----------|----------|----------|
| 19.9109 | glucose 2 | 0.402648 | 0.35161727 | 0.015901111 | 1.41601 | 8.94E-05 | 0.000561 | 1.42728 | 9.06E-05 | 0.035262 |
| 32.1784 | salicin | 0.385347 | 0.37268431 | 0.055201636 | 1.40203 | 0.000113674 | 0.006015 | 1.28275 | 0.000214 | 0.108973 |
| 16.0655 | fructose 1 | 3.83E-01 | 0.39346913 | 1.169566316 | 1.22368 | 0.001233505 | 1.712108 | 1.1115 | 0.002767 | 1.463883 |
| 31.7784 | Galactinol 1 | 3.71E-01 | 0.43318356 | 3.148983614 | 1.20986 | 0.000683894 | 0.103566 | 1.34653 | 0.000384 | 0.032889 |
| 23.106 | myo-inositol | 3.69E-01 | 0.40029752 | 0.860890351 | 1.10457 | 0.004440639 | 0.088772 | 1.13478 | 0.004759 | 0.103117 |
| 11.8561 | Glucose-1-phosphate | 3.69E-01 | 0.41322611 | 0.970552125 | 1.4404 | 4.77E-06 | 0.483273 | 1.45248 | 1.23E-05 | 0.497936 |
| 14.7657 | Glucose-1-phosphate | 0.352003 | 0.43638285 | 2.066403011 | 1.35322 | 5.12E-05 | 0.124775 | 1.44391 | 2.15E-05 | 0.060383 |
| 13.0622 | asparagine 5 | 0.3516 | 0.43386402 | 1.262288764 | 1.4356 | 0.000215437 | 44.31293 | 1.40888 | 0.000171 | 35.10522 |
| 10.4456 | 4-Vinylphenol dimer | 0.34762 | 0.44864873 | 0.998086809 | 1.35827 | 9.58E-05 | 2.190831 | 1.53253 | 1.49E-07 | 2.195031 |
| 20.3085 | sorbitol | 2.65E-01 | 0.57173061 | 1.302602315 | 1.28101 | 7.47E-04 | 14.49304 | 1.47706 | 1.33E-06 | 11.12622 |
| 27.0822 | 2-hydroxybutanoic acid | 2.54E-01 | 0.56743149 | 0.899446068 | 1.18071 | 0.001117621 | 0.340715 | 1.12938 | 0.002452 | 0.378806 |
| 12.6308 | L-dopa 2 | 0.252531 | 0.56396352 | 1.099711958 | 1.3749 | 2.06E-05 | 2.172187 | 1.151 | 0.001545 | 1.975233 |
| 15.2684 | ornithine | 0.240059 | 0.58867881 | 0.868337946 | 1.26974 | 0.002170712 | 302989.5 | 1.25817 | 0.001404 | 348930.4 |
| 26.3876 | N-Carbamylglutamate 2 | 2.22E-01 | 0.62215745 | 0.695241945 | 1.23502 | 0.001162558 | 0.019456 | 1.27028 | 0.001215 | 0.027984 |
| 12.5718 | 3-Methylthiopropylamine | 0.219235 | 0.63111401 | 1.040195189 | 1.35939 | 4.93E-04 | 1.525179 | 1.51598 | 7.69E-06 | 1.466243 |
| 8.05499 | 2-hydroxypyridine | 0.206602 | 0.6572129 | 0.958192971 | 1.05838 | 6.33E-03 | 2.23716 | 1.34672 | 4.85E-05 | 2.33477 |
| 25.4611 | ribulose-5-phosphate 2 | 0.188835 | 0.69259416 | 0.997497749 | 1.16335 | 0.001470127 | 0.556907 | 1.36022 | 0.000168 | 0.558304 |
| 29.1436 | Isopropyl-beta-D-thiogalactopyranoside | 0.188831 | 0.6628185 | 1.180825417 | 1.64224 | 4.74E-09 | 31.02626 | 1.18713 | 0.002795 | 26.27506 |
| 29.753 | xylitol | 0.180883 | 0.69514942 | 1.402820457 | 1.06758 | 0.003525407 | 0.541199 | 1.23525 | 0.000602 | 0.385794 |
| 22.9248 | 2-Monoolein | 1.73E-01 | 0.69026683 | 1.118238879 | 1.38347 | 3.55E-05 | 5.786756 | 1.14579 | 0.001515 | 5.174883 |
| 24.0887 | Glucose-1-phosphate | 0.159767 | 0.7267741 | 1.270845969 | 1.12828 | 0.00505797 | 12.58363 | 1.19116 | 0.001251 | 9.901776 |
| 17.8578 | 2-Deoxyerythritol | 1.38E-01 | 0.75670927 | 1.442945124 | 1.15256 | 0.001193003 | 0.361617 | 1.17643 | 0.000908 | 0.25061 |
| 28.4476 | lactose 1 | 0.115858 | 0.79078458 | 1.010534293 | 1.36238 | 2.95E-05 | 0.476172 | 1.12484 | 0.002224 | 0.471208 |
| 14.8882 | Glucose-1-phosphate | 0.105784 | 0.82337264 | 1.127635927 | 1.33199 | 6.55E-05 | 0.495963 | 1.49504 | 8.55E-06 | 0.439826 |
| 25.5091 | beta-Mannosylglycerate 1 | 0.084995 | 0.85082672 | 1.041502001 | 1.00125 | 0.007640822 | 0.792582 | 1.01161 | 0.008983 | 0.760999 |
| 8.98509 | oxalic acid | 0.051188 | 0.91179416 | 1.095589235 | 1.21042 | 2.56E-03 | 1.749788 | 1.39074 | 5.75E-05 | 1.597121 |
| 17.2629 | Carnitine | 3.32E-02 | 0.93970267 | 1.111379487 | 1.18095 | 0.001702684 | 0.112307 | 1.18049 | 0.00178 | 0.101052 |
| 23.0375 | myo-inositol | 0.008986 | 0.98442622 | 1.098728421 | 1.33821 | 4.70E-04 | 18.442 | 1.47937 | 6.73E-06 | 16.78486 |
| 26.1339 | Lactobionic Acid 1 | 0.019141 | 0.96560685 | 1.00108498 | 1.03583 | 0.008524386 | 1.439041 | 0.904798 | 0.021973 | 1.437482 |
| 27.5503 | ribitol | 0.177127 | 0.68667971 | 1.0137723 | 1.15232 | 0.003090668 | 7.544037 | 0.983886 | 0.013534 | 7.44155 |
| 10.427 | glycerol | 0.293351 | 0.4975311 | 0.75133521 | 1.10861 | 0.004929544 | 1.289492 | 0.530964 | 0.201859 | 1.716267 |
| 17.17681 | oxalic acid | 0.329233 | 0.46428345 | 1.10342932 | 1.0393 | 0.007279139 | 1.387189 | 0.889193 | 0.020672 | 1.257162 |
| 27.1557 | Glucose-1-phosphate | 0.35785 | 0.41013893 | 0.935561132 | 1.12786 | 0.005045333 | 10.32251 | 0.951224 | 0.019011 | 11.03349 |
| 17.6007 | Glucose-1-phosphate | 0.444768 | 0.31386297 | 0.861818902 | 1.14496 | 0.001322768 | 0.438647 | 0.954132 | 0.011367 | 0.508978 |
| 28.5346 | Diglycerol 2 | 5.21E-01 | 0.22834219 | 0.116050681 | 1.08242 | 0.005393405 | 0.040079 | 0.678521 | 0.085721 | 0.345355 |
| 24.9673 | 3-Hydroxynorvaline 2 | 5.34E-01 | 0.23551869 | 0.840545413 | 1.06913 | 0.003447509 | 0.559675 | 0.923159 | 0.016325 | 0.665848 |
| 27.3477 | Tagatose 2 | 0.555091 | 0.19727188 | 0.209912941 | 1.03493 | 0.006991786 | 0.079732 | 0.697071 | 0.077752 | 0.379833 |
| 17.8037 | glycerol | 6.54E-01 | 0.14508058 | 1.856741254 | 1.01962 | 0.014603176 | 4.950588 | 0.665086 | 0.099463 | 2.666278 |
| 9.16161 | oxalic acid | 0.674541 | 0.12448463 | 1.43347755 | 1.05031 | 0.012136232 | 1.723719 | 0.500435 | 0.224336 | 1.202473 |
| 8.33988 | malonic acid 1 | 0.699054 | 0.10499739 | 0.381395742 | 1.49733 | 4.46E-06 | 0.294418 | 0.31534 | 0.446598 | 0.77195 |
| 15.56 | flavin adenine degrad product | 0.706456 | 0.10487879 | 0.712347396 | 1.09766 | 0.005953533 | 0.588769 | 0.556709 | 0.170483 | 0.82652 |
| 29.246 | 4-nitrocatechol | 7.51E-01 | 0.07835709 | 0.131607047 | 1.32652 | 0.000211696 | 0.046504 | 0.976716 | 0.009191 | 0.353356 |
| 14.9805 | 5-Dihydrocortisol 1 | 7.68E-01 | 0.07004996 | 1.511568321 | 1.06974 | 0.003736073 | 2.121587 | 0.334985 | 0.412424 | 1.403567 |
| 13.9526 | trans-4-hydroxy-L-proline 2 | 0.832401 | 0.06491643 | 2.353565896 | 1.07949 | 0.006662985 | 7.132678 | 0.746606 | 0.05617 | 3.030584 |
| 27.3384 | xylitol | 0.885875 | 0.0381944 | 2.170656635 | 1.06676 | 0.005526823 | 4.105479 | 0.372533 | 0.360313 | 1.891353 |
| 29.1854 | Isopropyl-beta-D-thiogalactopyranoside | 9.29E-01 | 0.02524875 | 0.2252377 | 1.32353 | 6.80E-05 | 0.150576 | 0.590351 | 0.140794 | 0.668523 |

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|---------|-------------------------------|----------|------------|-------------|---------|-------------|----------|----------|----------|----------|
| 30.0828 | prunin degr. Prod. 2 | 0.948951 | 0.02154339 | 1.352250503 | 1.33509 | 0.00030916 | 1.440839 | 0.268384 | 0.517435 | 1.065512 |
| 12.5618 | aspartic acid 2 | 0.976075 | 0.01818346 | 1.477969257 | 1.52579 | 2.74E-07 | 2.192641 | 0.880062 | 0.026752 | 1.48355 |
| 28.3427 | Acetol 1 | 0.984375 | 0.02593074 | 5.516341594 | 1.11658 | 0.007092645 | 21.08607 | 0.503915 | 0.21581 | 3.822474 |
| 26.4271 | Analyte 354 | 1.01114 | 0.01613729 | 0.79130205 | 1.19266 | 0.000694325 | 0.634628 | 0.733838 | 0.062474 | 0.802005 |
| 23.0846 | Linoleic acid methyl ester | 1.03787 | 0.01423872 | 3.195005623 | 1.002 | 0.01828247 | 2.555324 | 0.230807 | 0.577624 | 0.799787 |
| 22.7804 | Methyl Palmitoleate | 1.06401 | 0.01045242 | 1.671271038 | 1.04868 | 0.009653015 | 1.594104 | 0.129922 | 0.752998 | 0.953827 |
| 8.10247 | lactic acid | 1.09067 | 0.0086077 | 0.570842872 | 1.06966 | 0.004030457 | 0.633108 | 0.244546 | 0.551334 | 1.109075 |
| 17.4188 | Glucose-1-phosphate | 1.09568 | 0.00978275 | 0.709538535 | 1.23141 | 0.000445632 | 0.578732 | 0.779126 | 0.04698 | 0.815646 |
| 11.1604 | D-Glyceric acid | 1.10128 | 0.01126714 | 1.581743319 | 1.08594 | 0.005218513 | 1.715624 | 0.276255 | 0.499379 | 1.084641 |
| 15.4537 | shikimic acid | 1.1466 | 0.0084628 | 1.591298441 | 1.04604 | 0.011966239 | 1.524341 | 0.192436 | 0.639802 | 0.957923 |
| 13.307 | oxalic acid | 1.18456 | 0.00494859 | 7.8769E-06 | 1.45075 | 4.58E-05 | 9E-06 | 0.169766 | 0.681415 | 1.142116 |
| 33.4768 | Analyte 426 | 1.18627 | 0.00304657 | 0.354822042 | 1.13175 | 0.002547406 | 0.268819 | 0.443092 | 0.275398 | 0.757617 |
| 11.5011 | fumaric acid | 1.20119 | 0.00442361 | 1.555367492 | 1.32388 | 0.000560404 | 1.84778 | 0.767586 | 0.051078 | 1.188002 |
| 20.739 | Dihydroxyacetone | 1.23326 | 0.00475203 | 6.068147497 | 1.28467 | 0.001831222 | 127.1998 | 0.734822 | 0.075669 | 20.96189 |
| 23.1448 | Linoleic acid methyl ester | 1.23658 | 0.00251727 | 1.506220228 | 1.23907 | 0.000742294 | 1.651242 | 0.33388 | 0.412701 | 1.096282 |
| 16.2662 | 2,2-Dimethylsuccinic Acid | 1.25E+00 | 0.00177452 | 1.542572695 | 1.31311 | 0.000552964 | 1.651539 | 0.285964 | 0.486645 | 1.070639 |
| 10.8128 | malonic acid 1 | 1.26E+00 | 0.00214812 | 1.673708686 | 1.07093 | 0.004124402 | 3.292968 | 0.684658 | 0.09545 | 1.967468 |
| 8.66405 | Maleimide | 1.30844 | 0.00054669 | 3.385992938 | 1.11326 | 0.004484672 | 1.867256 | 0.803081 | 0.045772 | 0.551465 |
| 30.4418 | Lactobionic Acid 1 | 1.34654 | 0.00037517 | 1.985904259 | 1.12205 | 0.003066103 | 4.653005 | 0.54428 | 0.181815 | 2.343016 |
| 20.2773 | Methyl Palmitoleate | 1.35E+00 | 0.00084204 | 1.53523943 | 1.25111 | 0.00043247 | 1.645107 | 0.266513 | 0.5155 | 1.071564 |
| 25.1783 | Threitol | 1.35E+00 | 0.00093195 | 1.797476309 | 1.1986 | 0.002508092 | 1.64913 | 0.408836 | 0.31462 | 0.91747 |
| 24.2136 | Linoleic acid methyl ester | 1.36E+00 | 0.00083188 | 1.782900463 | 1.01023 | 0.009939452 | 1.434117 | 0.688109 | 0.081384 | 0.804373 |
| 18.3135 | mucic acid | 1.37442 | 0.00047036 | 1.616048616 | 1.30462 | 0.000240513 | 1.704298 | 0.200898 | 0.624234 | 1.054608 |
| 20.7043 | coniferyl alcohol | 1.39E+00 | 0.0003522 | 0.437132149 | 1.45511 | 5.12E-06 | 0.32579 | 0.993353 | 0.007825 | 0.745289 |
| 25.3544 | beta-Mannosylglycerate 1 | 1.39E+00 | 0.00016435 | 0.506301821 | 1.12079 | 0.002573006 | 0.439961 | 0.313736 | 0.445203 | 0.868971 |
| 9.52459 | Norleucine 2 | 1.40215 | 0.0002195 | 2.882999006 | 1.14581 | 0.004669343 | 1.877909 | 0.915695 | 0.019798 | 0.651373 |
| 25.0877 | Androstanediol | 1.41244 | 0.00010365 | 3.09565194 | 1.13231 | 0.001564539 | 2.320197 | 0.287651 | 0.481749 | 0.749502 |
| 18.894 | glucuronic acid 2 | 1.47291 | 0.00039468 | 6.213288888 | 1.42932 | 0.00016573 | 20.88125 | 0.763979 | 0.051139 | 3.36074 |
| 23.3911 | Methyl Palmitoleate | 1.48323 | 8.49E-05 | 1.789344948 | 1.27975 | 0.000259016 | 1.671504 | 0.238707 | 0.56032 | 0.934143 |
| 31.0634 | Monoolein | 1.48937 | 0.00011417 | 1.521581522 | 1.33072 | 0.000206153 | 1.475279 | 0.215614 | 0.598912 | 0.96957 |
| 31.4025 | malonic acid 1 | 1.53232 | 2.33E-05 | 0.677084838 | 1.06166 | 0.004161411 | 0.838224 | 0.977316 | 0.00921 | 1.23799 |
| 19.4509 | N-Acetyl-beta-D-mannosamine 2 | 1.54311 | 0.00015971 | 18.7254757 | 1.44169 | 0.000144868 | 35.31879 | 0.219532 | 0.59257 | 1.886136 |
| 11.5696 | serine 1 | 1.55E+00 | 0.00010158 | 2.11492903 | 1.44808 | 3.23E-05 | 2.335774 | 0.472031 | 0.243548 | 1.104422 |

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|---------|----------------------------|----------|------------|-------------|------------------------|-------------|----------|----------------------|----------|----------|
| 14.6164 | conduritol b epoxide 1 | 1.56E+00 | 6.68E-06 | 4.484487246 | 1.32999 | 6.94E-05 | 2.444073 | 0.61816 ₈ | 0.120278 | 0.545006 |
| 20.6378 | tyrosine 1 | 1.56697 | 3.39E-05 | 2.351600637 | 1.21203 | 0.000968884 | 1.742694 | 0.96681 ₆ | 0.010756 | 0.741067 |
| 28.3005 | beta-Mannosylglycerate 2 | 1.57E+00 | 4.46E-05 | 1.844547037 | 1.49979 | 5.11E-06 | 2.158626 | 0.8292 | 0.03231 | 1.170274 |
| 15.646 | phenylalanine 1 | 1.63E+00 | 1.00E-05 | 2.15763739 | 1.43282 | 1.44E-05 | 2.001156 | 0.35016 ₄ | 0.391975 | 0.927476 |
| 30.7118 | Monoolein | 1.63374 | 2.80E-07 | 4.796244233 | 1.49466 | 1.44E-06 | 3.010038 | 0.64286 ₇ | 0.106734 | 0.627582 |
| 24.6284 | Galactinol 3 | 1.63967 | 2.89E-07 | 7.208434669 | 1.29534 | 0.000191466 | 2.710716 | 0.55219 ₄ | 0.169684 | 0.376048 |
| 10.7963 | Isoleucine | 1.64E+00 | 9.19E-06 | 2.768184725 | 1.51926 | 2.82E-05 | 2.585397 | 0.40706 | 0.320455 | 0.933968 |
| 28.5472 | 1-Monopalmitin | 1.70E+00 | 1.77E-06 | 2.571421716 | 1.5909 | 1.31E-06 | 2.809125 | 0.67674 ₉ | 0.087057 | 1.092441 |
| 9.8543 | valine | 1.70707 | 2.83E-06 | 3.278162573 | 1.57943 | 3.20E-06 | 3.336878 | 0.11306 ₂ | 0.783367 | 1.017911 |
| 31.5851 | beta-Mannosylglycerate 1 | 1.67794 | 5.24E-07 | 0.441363467 | 0.702154 | 0.077611067 | 0.274553 | 0.40244 ₈ | 0.333989 | 0.622056 |
| 26.9392 | Linoleic acid methyl ester | 1.47721 | 0.00071183 | 67387.38291 | 0.397226 | 0.319233711 | 0.392984 | 0.61449 ₄ | 0.139501 | 5.83E-06 |
| 34.2067 | shikimic acid | 1.45682 | 0.00017368 | 0.463374058 | 0.638828 | 0.108692106 | 0.362449 | 0.23623 ₁ | 0.570176 | 0.782196 |
| 29.832 | xylitol | 1.38E+00 | 0.0002334 | 2.307519835 | 0.269831 | 0.499015821 | 1.372717 | 0.47811 ₃ | 0.245099 | 0.594888 |
| 21.3934 | isocitric acid 2 | 1.33403 | 0.00113882 | 1.540900361 | 0.366352 | 0.364522644 | 1.151034 | 0.79559 ₈ | 0.048196 | 0.746988 |
| 28.0328 | 2-Monoolein | 1.31E+00 | 0.0013555 | 2.710829685 | 0.486404 | 0.229377973 | 1.337412 | 0.84856 ₄ | 0.031593 | 0.493359 |
| 12.0893 | 22-Ketocholesterol | 1.29854 | 0.00097073 | 0.333614867 | 0.18025 | 0.65909952 | 0.724331 | 0.98738 ₄ | 0.009888 | 2.171159 |
| 12.9037 | fucose 1 | 1.27694 | 0.00235893 | 0.371716041 | 0.8938 | 0.019209107 | 0.309203 | 0.28290 ₃ | 0.495676 | 0.831825 |
| 24.0025 | beta-Mannosylglycerate 1 | 1.27E+00 | 0.00230367 | 2.507318332 | 0.552013 | 0.171499153 | 1.328785 | 0.76161 ₂ | 0.055924 | 0.529963 |
| 30.6436 | Lactobionic Acid 1 | 1.27202 | 0.0010497 | 1.476899238 | 0.56684 | 0.154547526 | 0.651754 | 0.81413 | 0.048022 | 0.441299 |
| 9.01093 | cycloleucine 1 | 1.22906 | 0.0022494 | 0.549399649 | 0.988706 | 0.008122564 | 0.701677 | 0.60726 ₁ | 0.130301 | 1.27717 |
| 11.9577 | Methylmalonic acid | 1.2004 | 0.00574713 | 0.496765927 | 0.651601 | 0.105995575 | 0.645612 | 0.59937 ₅ | 0.139152 | 1.29963 |
| 16.7707 | Threitol | 1.16396 | 0.00638663 | 2.600389509 | 0.932201 | 0.024091313 | 1.916662 | 0.50584 ₃ | 0.209438 | 0.737067 |
| 20.9699 | Glucose-1-phosphate | 1.16309 | 0.00471881 | 0.156282093 | 0.924709 | 0.018154071 | 0.127834 | 0.21149 ₅ | 0.607237 | 0.817968 |
| 10.5093 | Ethanolamine | 1.10808 | 0.00923741 | 1.321583256 | 0.0036288 ₇ | 0.992992283 | 1.036302 | 0.96927 ₇ | 0.011979 | 0.784137 |
| 29.8614 | D-erythro-sphingosine 1 | 1.09387 | 0.00714385 | 0.638483445 | 0.995151 | 0.007871087 | 0.515781 | 0.43072 ₈ | 0.292309 | 0.807823 |
| 24.7284 | cis-gondoic acid | 1.06787 | 0.02271678 | 13.51946749 | 0.917928 | 0.032940423 | 6.307265 | 0.40076 ₂ | 0.328384 | 0.466532 |
| 18.638 | 3,4-dihydroxybenzoic acid | 1.06039 | 0.00920308 | 0.762640986 | 0.753298 | 0.05298224 | 0.7308 | 0.10903 ₉ | 0.791908 | 0.958249 |
| 24.6826 | cis-gondoic acid | 1.05745 | 0.01452262 | 0.42945853 | 0.770076 | 0.071448765 | 0.524049 | 0.64454 ₂ | 0.107424 | 1.220256 |
| 29.2258 | beta-Mannosylglycerate 2 | 1.05E+00 | 0.01157183 | 0.826590563 | 0.566245 | 0.165480064 | 0.93503 | 0.59113 ₆ | 0.138438 | 1.131188 |
| 21.8319 | malonic acid 1 | 1.04888 | 0.00966449 | 1.83297795 | 0.133062 | 0.740072049 | 0.821682 | 0.74331 ₉ | 0.062032 | 0.448277 |
| 15.0594 | Glucose-1-phosphate | 1.03926 | 0.0246798 | 2.460289871 | 0.347039 | 0.385709626 | 0.683955 | 0.80097 ₄ | 0.052144 | 0.277998 |
| 20.6532 | ascorbate | 1.03116 | 0.01778891 | 1.838265269 | 0.167913 | 0.677863798 | 1.211797 | 0.49192 ₆ | 0.232576 | 0.659207 |
| 32.9689 | Galactinol 1 | 1.02E+00 | 0.01603559 | 0.621553196 | 0.873035 | 0.02415806 | 1.011609 | 0.67478 ₇ | 0.097044 | 1.62755 |

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|---------|--------------------------------|----------|------------|-------------|-----------|-------------|----------|----------|----------|----------|
| 16.6802 | ribitol | 1.00891 | 0.01475694 | 0.272260177 | 0.298368 | 0.456029983 | 0.399813 | 0.261371 | 0.527381 | 1.468496 |
| 13.2787 | glutamine 3 | 1.00058 | 0.03074937 | 8.018095247 | 0.929707 | 0.029799519 | 8.431703 | 0.021094 | 0.959117 | 1.051584 |
| 9.61065 | oxalic acid | 0.991803 | 0.03005245 | 5.494022594 | 0.950528 | 0.025132254 | 6.511097 | 0.094141 | 0.819012 | 1.185124 |
| 10.076 | N-(3-aminopropyl)-morpholine 2 | 0.977866 | 0.03373546 | 6.968537764 | 0.987027 | 0.02009309 | 16.10489 | 0.332758 | 0.414706 | 2.311085 |
| 18.9427 | Dehydroascorbic Acid 2 | 9.72E-01 | 0.03367597 | 3.416279507 | 0.136971 | 0.73741998 | 0.777364 | 0.836144 | 0.039866 | 0.227547 |
| 19.3525 | Tagatose 1 | 9.50E-01 | 0.02363423 | 3.182300128 | 0.937763 | 0.014542766 | 3.957303 | 0.084794 | 0.836656 | 1.243535 |
| 8.48201 | 2-Butyne-1,4-diol | 9.48E-01 | 0.045435 | 10.07285972 | 0.842838 | 0.049693527 | 8.871339 | 0.045364 | 0.912924 | 0.880717 |
| 26.1229 | Threitol | 9.16E-01 | 0.04080818 | 1.54879975 | 0.174558 | 0.676407013 | 1.102886 | 0.758703 | 0.055669 | 0.712091 |
| 23.6056 | 2-Monoolein | 0.899027 | 0.03278078 | 1.529690001 | 0.145935 | 0.717430636 | 1.074345 | 0.447235 | 0.273864 | 0.702329 |
| 10.6752 | thymidine 3 | 0.883229 | 0.05428264 | 1.324208951 | 0.239379 | 0.560614201 | 1.09441 | 0.50364 | 0.220733 | 0.826463 |
| 9.33708 | 4-HYDROXYPYRIDINE | 8.80E-01 | 0.03686953 | 1.950331365 | 0.521898 | 0.196109665 | 1.494375 | 0.34745 | 0.393596 | 0.766216 |
| 17.8392 | 3,6-Anhydro-D-galactose 2 | 0.867335 | 0.05179989 | 2.024040402 | 0.398874 | 0.327205271 | 1.532213 | 0.314924 | 0.443987 | 0.757007 |
| 14.3115 | Prostaglandin E2 2 | 0.824242 | 0.06745214 | 4.815306829 | 0.140703 | 0.738025959 | 1.100322 | 0.976423 | 0.010299 | 0.228505 |
| 29.9568 | Tagatose 1 | 0.818354 | 0.05191688 | 4.164358027 | 0.488314 | 0.224423937 | 1.941637 | 0.340502 | 0.40345 | 0.466251 |
| 27.3209 | lactose 1 | 8.03E-01 | 0.07945546 | 0.763151959 | 0.855903 | 0.025280471 | 0.526615 | 0.599766 | 0.145407 | 0.690053 |
| 37.9128 | Galactinol 3 | 0.803187 | 0.05790108 | 0.871649641 | 0.706349 | 0.07165224 | 0.796084 | 0.298582 | 0.468277 | 0.913307 |
| 26.4567 | Tagatose 1 | 0.797501 | 0.05900983 | 1.217705832 | 0.164125 | 0.682529844 | 0.986411 | 0.669237 | 0.091315 | 0.810057 |
| 23.0188 | myo-inositol | 0.776585 | 0.07934242 | 0.881252651 | 0.0994779 | 0.806301977 | 0.977553 | 0.412303 | 0.31607 | 1.109276 |
| 16.5485 | Ribonic acid, gamma-lactone | 0.759672 | 0.07661768 | 0.850404986 | 0.935968 | 0.01320789 | 0.772685 | 0.387088 | 0.340764 | 0.908608 |
| 26.3769 | fructose 2 | 0.74946 | 0.07803036 | 1.226131815 | 0.750667 | 0.053520164 | 1.350109 | 0.238813 | 0.56061 | 1.101113 |
| 23.6844 | 5-alpha-Dihydroprogesterone 2 | 0.742266 | 0.10461771 | 4.72703645 | 0.092847 | 0.82913489 | 1.004948 | 0.847736 | 0.027737 | 0.212596 |
| 29.3555 | 2-Monoolein | 0.716652 | 0.09228551 | 0.668782448 | 0.198461 | 0.619513091 | 1.411309 | 0.554618 | 0.170869 | 2.110266 |
| 22.1797 | oxalic acid | 0.712356 | 0.09457234 | 0.715502357 | 0.4353 | 0.284733994 | 0.795414 | 0.342659 | 0.401395 | 1.111687 |
| 25.0688 | Glucose-1-phosphate | 7.06E-01 | 0.11423641 | 1.492203681 | 0.192518 | 0.637920022 | 1.267312 | 0.358073 | 0.382791 | 0.849289 |
| 25.7316 | beta-Mannosylglycerate 1 | 0.700966 | 0.10139823 | 1.993341371 | 0.813679 | 0.040242333 | 0.175737 | 0.818481 | 0.047444 | 0.088162 |
| 22.94 | conduritol b epoxide 2 | 6.98E-01 | 0.10751942 | 0.497316938 | 0.236287 | 0.576270105 | 1.709715 | 0.900393 | 0.019008 | 3.437878 |
| 20.4278 | glucuronic acid 3 | 0.694341 | 0.11171857 | 1.223115212 | 0.465999 | 0.244690018 | 0.927185 | 0.898226 | 0.020421 | 0.758052 |
| 19.2152 | quinic acid | 0.687765 | 0.12381704 | 3.15119397 | 0.552097 | 0.183284423 | 2.506795 | 0.11758 | 0.774835 | 0.795506 |
| 15.3851 | flavin adenine degrad product | 0.66949 | 0.15260097 | 1.420033645 | 0.564277 | 0.17258431 | 1.456331 | 0.054232 | 0.895669 | 1.025561 |
| 26.372 | Galactinol 3 | 6.62E-01 | 0.14833945 | 3.255892462 | 0.408686 | 0.314150252 | 0.578681 | 0.918562 | 0.019838 | 0.177733 |
| 12.9006 | Diglycerol 2 | 0.648241 | 0.16032011 | 2.703862761 | 0.153152 | 0.705011696 | 1.582933 | 0.206586 | 0.61902 | 0.585434 |
| 8.59009 | Analyte 14 | 0.631418 | 0.14143767 | 0.313463958 | 0.0797406 | 0.849818001 | 1.078843 | 0.674507 | 0.093045 | 3.44168 |
| 10.2694 | 4-Hydroxyphenylethanol | 6.21E-01 | 0.1869173 | 1.360978181 | 0.567037 | 0.185238419 | 1.370466 | 0.033472 | 0.935229 | 1.006971 |

| | | | | | | | | | | |
|---------|----------------------------------|----------|------------|--------------|-----------|-------------|----------|----------|----------|----------|
| 13.4095 | L-Malic acid | 0.620257 | 0.15111145 | 0.033906006 | 0.332394 | 0.404614397 | 0.114708 | 0.407259 | 0.320566 | 3.383124 |
| 17.0185 | MALONAMIDE 5 | 0.615575 | 0.16980323 | 2.038654405 | 0.371443 | 0.37293856 | 1.477697 | 0.23462 | 0.566852 | 0.724839 |
| 15.0466 | 2-Monopalmitin | 0.610534 | 0.1604665 | 1.63243271 | 0.833166 | 0.030417875 | 3.701396 | 0.370426 | 0.362444 | 2.267411 |
| 12.7293 | malonic acid 1 | 0.609686 | 0.15548479 | 1.857315136 | 0.446665 | 0.301753844 | 0.935892 | 0.829215 | 0.042195 | 0.503895 |
| 13.5196 | L-Malic acid | 0.607761 | 0.15956353 | 0.020197004 | 0.398339 | 0.317950417 | 0.066352 | 0.392326 | 0.34009 | 3.285215 |
| 32.2212 | Epicatechin | 0.586147 | 0.1850495 | 1.687267701 | 0.366359 | 0.365417343 | 0.647011 | 0.781465 | 0.046646 | 0.383467 |
| 15.2818 | glutamic acid | 5.78E-01 | 0.18512638 | 1.516233846 | 0.120575 | 0.780381866 | 1.108441 | 0.733072 | 0.068092 | 0.731049 |
| 13.9112 | lactic acid | 0.566676 | 0.21779722 | 1.282578134 | 0.058977 | 0.890326548 | 1.107765 | 0.623339 | 0.117208 | 0.863702 |
| 16.4343 | Diglycerol 2 | 5.40E-01 | 0.26302899 | 13.26610731 | 0.410687 | 0.356609496 | 3.871398 | 0.85186 | 0.028945 | 0.291826 |
| 11.8735 | cycloleucine 1 | 0.519746 | 0.26487087 | 1.132092881 | 0.904306 | 0.021008271 | 1.445033 | 0.809056 | 0.039923 | 1.276427 |
| 26.0748 | N-epsilon-Acetyl-L-lysine 1 | 0.514822 | 0.26342595 | 1.366508502 | 0.236382 | 0.58566898 | 0.94436 | 0.957495 | 0.011156 | 0.691075 |
| 16.5558 | 3,6-Anhydro-D-galactose 2 | 5.14E-01 | 0.24622884 | 0.727866992 | 0.957004 | 0.011636092 | 0.488036 | 0.652749 | 0.099295 | 0.670502 |
| 12.0819 | malonic acid 1 | 0.507945 | 0.27626924 | 1.419196193 | 0.928149 | 0.01703244 | 3.544314 | 0.856924 | 0.028741 | 2.497409 |
| 17.9573 | 2-Deoxytetronic acid | 0.502618 | 0.26388759 | 1.255835191 | 0.165538 | 0.680687505 | 1.165393 | 0.083184 | 0.841107 | 0.927982 |
| 20.0629 | myo-inositol | 0.495525 | 0.25079063 | 0.348676947 | 0.440055 | 0.269799742 | 0.124368 | 0.341679 | 0.41059 | 0.356686 |
| 13.5748 | glycine 1 | 0.494696 | 0.25214568 | 0.120091025 | 0.336894 | 0.405896741 | 0.428823 | 0.39742 | 0.338723 | 3.570813 |
| 18.816 | Allo-inositol | 0.484522 | 0.26858314 | 1.168777206 | 0.283822 | 0.477655829 | 0.805775 | 0.491684 | 0.230947 | 0.689417 |
| 10.2007 | 3-hydroxypyruvate | 0.475438 | 0.2839966 | 0.8679433580 | 0.0917531 | 0.833476101 | 1.047408 | 0.648892 | 0.109598 | 1.20677 |
| 26.6112 | cytidine-monophosphate degr prod | 0.469259 | 0.31931971 | 1.3285898570 | 0.0726954 | 0.862485018 | 1.005371 | 0.576069 | 0.157197 | 0.75672 |
| 14.7398 | Glucose-1-phosphate | 0.459271 | 0.30409568 | 1.262870255 | 0.462366 | 0.245477717 | 2.367075 | 0.34 | 0.412652 | 1.874361 |
| 34.8666 | 3-Phenyllactic acid | 0.448352 | 0.32332993 | 1.14692811 | 0.645137 | 0.139853162 | 1.201418 | 0.238157 | 0.565336 | 1.047509 |
| 30.3167 | cellobiose 2 | 4.48E-01 | 0.31142335 | 1.194435296 | 0.571764 | 0.14985131 | 0.792863 | 0.840668 | 0.030286 | 0.663798 |
| 8.14825 | Analyte 5 | 0.443996 | 0.3081344 | 0.876707493 | 0.529399 | 0.199427369 | 5.039431 | 0.782448 | 0.049051 | 5.748133 |
| 17.4465 | MALONAMIDE 5 | 4.44E-01 | 0.33197747 | 1.516025048 | 0.187898 | 0.651990344 | 1.146506 | 0.213602 | 0.603069 | 0.756258 |
| 11.2441 | nicotinic acid | 0.439219 | 0.34094844 | 1.34403381 | 0.497078 | 0.251915228 | 1.380592 | 0.101537 | 0.805412 | 1.0272 |
| 29.5274 | fructose 1 | 0.433435 | 0.31595306 | 0.716723466 | 0.619682 | 0.115972817 | 1.301945 | 0.551132 | 0.182807 | 1.816523 |
| 13.1786 | Methylmalonic acid | 0.408858 | 0.34424329 | 0.00669034 | 0.397518 | 0.318952222 | 0.024401 | 0.283596 | 0.494607 | 3.647146 |
| 24.0883 | Phytol | 4.07E-01 | 0.36707963 | 1.451193484 | 0.480451 | 0.228133146 | 0.840068 | 0.721245 | 0.072748 | 0.578881 |
| 22.985 | myo-inositol | 3.88E-01 | 0.3784258 | 0.603954589 | 0.534957 | 0.178782679 | 0.479514 | 0.234103 | 0.56795 | 0.793957 |
| 17.7438 | creatine degr | 3.82E-01 | 0.41279624 | 1.171209138 | 0.22888 | 0.592265346 | 0.945242 | 0.772802 | 0.047798 | 0.807065 |
| 32.6047 | Epicatechin | 0.377422 | 0.3973852 | 1.016459511 | 0.158149 | 0.696352171 | 1.047234 | 0.099359 | 0.809659 | 1.030276 |
| 28.8321 | 2-Monoolein | 0.374521 | 0.43861682 | 3.630635605 | 0.242018 | 0.575374764 | 2.288972 | 0.154023 | 0.711749 | 0.63046 |
| 17.3715 | Diglycerol 2 | 0.356486 | 0.43903553 | 0.948321001 | 0.101656 | 0.811685295 | 1.060218 | 0.546072 | 0.173096 | 1.117995 |
| 33.7096 | raffinose | 0.343539 | 0.42711225 | 0.893763475 | 0.399312 | 0.316626919 | 0.741058 | 0.197226 | 0.631998 | 0.829143 |

| | | | | | | | | | | |
|---------|--------------------------|----------|------------|-------------|-----------|-------------|----------|--------------|----------|----------|
| 15.8321 | Lyxose 1 | 0.33703 | 0.4527282 | 1.049522316 | 0.886157 | 0.020183558 | 0.910593 | 0.72664 4 | 0.064684 | 0.867627 |
| 22.9955 | 2-Monoolein | 0.335193 | 0.46990382 | 1.507746204 | 0.661509 | 0.127740423 | 5.21899 | 0.56792 8 | 0.161124 | 3.461452 |
| 21.3902 | 2-Hydroxyvaleric acid | 0.299484 | 0.49541794 | 0.652820216 | 0.448567 | 0.310034672 | 5.704983 | 0.61475 2 | 0.138033 | 8.73898 |
| 24.233 | Turanose 2 | 2.88E-01 | 0.52976986 | 0.895364158 | 0.291935 | 0.487730452 | 1.22215 | 0.64232 9 | 0.105352 | 1.364975 |
| 12.158 | Analyte 80 | 0.268844 | 0.5555686 | 1.205513296 | 0.53866 | 0.204788476 | 1.38654 | 0.34105 9 | 0.404037 | 1.150166 |
| 9.9618 | L-Threose 1 | 0.253663 | 0.5981273 | 1.857975482 | 0.373504 | 0.379060386 | 0.868558 | 0.91317 8 | 0.02278 | 0.467476 |
| 24.557 | aspartic acid 2 | 0.237975 | 0.5926497 | 0.992252288 | 0.870431 | 0.029338403 | 1.539551 | 0.96404 8 | 0.012144 | 1.551573 |
| 25.3283 | Dehydroepiandrosterone | 2.22E-01 | 0.61290203 | 0.957380128 | 0.265426 | 0.515135857 | 1.187587 | 0.39545 4 | 0.330989 | 1.240455 |
| 19.1288 | quinic acid | 1.97E-01 | 0.65734202 | 1.31395482 | 0.287947 | 0.518462203 | 1.313138 | 0.0012 | 0.997705 | 0.999378 |
| 17.621 | 2-Deoxyerythritol | 0.197047 | 0.65728138 | 1.013936364 | 0.790811 | 0.042668974 | 0.32213 | 0.72890 4 | 0.069926 | 0.317702 |
| 19.4677 | Lyxose 2 | 0.181612 | 0.68359593 | 0.757341511 | 0.0386115 | 0.924527441 | 0.855942 | 0.10199 5 | 0.804232 | 1.130193 |
| 29.0045 | sucrose | 1.79E-01 | 0.70389441 | 0.78893569 | 0.150225 | 0.720107047 | 1.065689 | 0.38752 1 | 0.344385 | 1.350793 |
| 10.8372 | threonine 2 | 1.74E-01 | 0.69751891 | 1.02009548 | 0.647716 | 0.102004551 | 0.518683 | 0.62853 6 | 0.126859 | 0.508465 |
| 9.22394 | p-cresol | 0.17295 | 0.70353695 | 1.409801339 | 0.479882 | 0.26967312 | 0.852988 | 0.72961 1 | 0.070228 | 0.605041 |
| 20.959 | beta-Mannosylglycerate 1 | 1.69E-01 | 0.70315716 | 0.786495794 | 0.523903 | 0.188741224 | 0.14695 | 0.52666 | 0.205241 | 0.186842 |
| 23.4071 | glucose 2 | 0.167569 | 0.70681159 | 0.994862506 | 0.350805 | 0.381970256 | 1.239506 | 0.44912 3 | 0.269382 | 1.245907 |
| 30.1755 | 2-Monoolein | 0.161264 | 0.72074716 | 1.323217376 | 0.340069 | 0.404438808 | 0.646794 | 0.47912 7 | 0.235545 | 0.488804 |
| 19.4666 | fructose 1 | 0.149895 | 0.73708757 | 0.728782768 | 0.211628 | 0.608794521 | 0.671739 | 0.06217 1 | 0.879894 | 0.921728 |
| 11.0543 | succinic acid | 1.47E-01 | 0.74934741 | 0.988365221 | 0.167729 | 0.692233916 | 1.043845 | 0.36543 4 | 0.369017 | 1.056133 |
| 25.6183 | creatine degr | 0.145371 | 0.76129233 | 1.113345743 | 0.433546 | 0.315985227 | 0.852191 | 0.99815 1 | 0.008314 | 0.765432 |
| 11.0339 | glycine 2 | 1.43E-01 | 0.75508909 | 1.013298876 | 0.598244 | 0.138827748 | 0.904063 | 0.57733 8 | 0.149543 | 0.892198 |
| 16.0642 | Glucose-1-phosphate | 0.137137 | 0.76863393 | 1.100914501 | 0.433723 | 0.283120788 | 0.466985 | 0.60076 | 0.139308 | 0.424179 |
| 17.6911 | Galactonic acid | 0.13667 | 0.77222461 | 0.860372715 | 0.279811 | 0.495007048 | 0.784053 | 0.24523 9 | 0.553383 | 0.911294 |
| 18.5355 | fucose 2 | 0.101468 | 0.82756788 | 1.062778555 | 0.719661 | 0.078663614 | 1.321714 | 0.84402 4 | 0.028493 | 1.243641 |
| 8.262 | oxalic acid | 9.90E-02 | 0.821488 | 0.999584928 | 0.803156 | 0.041086976 | 2.438592 | 0.50504 6 | 0.214898 | 2.439605 |
| 19.6895 | galactose 1 | 9.08E-02 | 0.83590345 | 1.082021063 | 0.859326 | 0.029861487 | 0.140145 | 0.88385 | 0.031307 | 0.129522 |
| 18.1714 | xylitol | 4.36E-02 | 0.92173818 | 0.964010547 | 0.407962 | 0.306228379 | 0.233589 | 0.43135 3 | 0.298662 | 0.24231 |
| 14.7195 | 2-Deoxyerythritol | 0.028304 | 0.950941 | 0.879978725 | 0.229985 | 0.564591502 | 0.496798 | 0.23598 7 | 0.571018 | 0.564557 |
| 23.4954 | glucose 2 | 0.01723 | 0.96920149 | 1.044041751 | 0.455159 | 0.254104026 | 1.310432 | 0.43908 6 | 0.280302 | 1.255153 |
| 18.7332 | isocitric acid 2 | 0.016724 | 0.97156188 | 1.299012822 | 0.461431 | 0.280251985 | 2.668975 | 0.70493 3 | 0.073047 | 2.054618 |
| 19.1628 | quinic acid | 1.28E-02 | 0.97674168 | 0.936714227 | 0.84936 | 0.032019728 | 7.64E-05 | 0.88294 | 0.032019 | 8.16E-05 |

Table S2. 142 metabolites varied among the three groups.

| | RT | Names | PubChem | KEGG | Relative Contents (N) | Relative Contents (O) | Relative Contents (T) | VIP | p-value | FC(T/O) | VIP | p-value | FC (T/N) | VIP | p-value | FC(O/N) |
|----|-------------|--------------------------------------|---------|--------|-----------------------------|-----------------------------|-----------------------------|--------------|--------------|----------|-------------|----------|----------|-------------|----------|----------|
| 1 | 15.217 3 | (+)- Dihydroc arveol 1,5- | | | 2.607771 | 2.2E-05 | 2.320482 | 1.666 15 | 2.72E- 05 | 105338.1 | N | N | N | 1.6655 7 | 5.82E-08 | 8.45E-06 |
| 2 | 10.815 | Anhydrogl ucitol 1- | 64960 | C07326 | 26.92387 | 1.72397 6 | 3.905063 | N | N | N | 1.5193 1 | 5.53E-07 | 0.145041 | 1.6342 7 | 4.91E-10 | 0.064032 |
| 3 | 14.341 1 | Hydroxya nthraquino ne 1 1- | | | 3.516376 | 4.57345 8 | 6.093776 | N | N | N | 1.1904 2 | 0.003502 | 1.732971 | 1.0361 5 | 0.006514 | 1.300617 |
| 4 | 28.547 2 | Monopalmitin 2,2- | | | 4.057147 | 4.43219 2 | 11.39703 | 1.70E +00 | 1.77E- 06 | 2.571422 | 1.5909 | 1.31E-06 | 2.809125 | N | N | N |
| 5 | 16.266 2 | Dimethylsuccinic Acid 22- | 11701 | | 67.45561 | 72.2206 3 | 111.4056 | 1.25E +00 | 0.00177 5 | 1.542573 | 1.3131 1 | 0.000553 | 1.651539 | N | N | N |
| 6 | 12.089 3 | Ketocholesterol 2- | 91474 | | 1.409354 | 3.05993 2 | 1.020839 | 1.298 54 | 0.00097 1 | 0.333615 | N | N | N | N | N | N |
| 7 | 10.648 8 | Deoxyerythritol 2- | | | 3.714874 | 1.16495 | 4.625451 | 1.616 33 | 3.50E- 05 | 3.970516 | N | N | N | 1.6273 5 | 7.88E-10 | 0.313591 |
| 8 | 27.082 2 | hydroxybutanoic acid 2- | 11266 | C05984 | 25.51174 | 9.66399 9 | 8.692246 | N | N | N | 1.1807 1 | 0.001118 | 0.340715 | 1.1293 8 | 0.002452 | 0.378806 |
| 9 | 8.0549 9 | hydroxyproline 2- | 72924 | C01020 | 26.74934 | 62.4535 7 | 59.84257 | N | N | N | 1.0583 8 | 6.33E-03 | 2.23716 | 1.3467 2 | 4.85E-05 | 2.33477 |
| 10 | 20.033 7 | 2-Keto-L-gulonic acid | 440390 | | 1.41E-05 | 3.10997 5 | 1.157918 | 1.193 02 | 0.00811 | 0.372324 | N | N | N | 1.6929 5 | 2.78E-09 | 220646.7 |
| 11 | 24.133 7 | 2-Monoolein 3,4- | | | 5.995023 | 3.19296 7 | 10.08739 | 1.50E +00 | 0.00032 2 | 3.159254 | 1.0075 9 | 0.010305 | 1.682628 | 1.0928 2 | 0.004162 | 0.532603 |
| 12 | 18.638 | dihydroxybenzoic acid 3,6- | | | 8.281953 | 7.93617 3 | 6.052451 | 1.060 39 | 0.00920 3 | 0.762641 | N | N | N | N | N | N |
| 13 | 14.589 1 | Anhydro-D-galactose 1 3- | | C06474 | 7.185193 | 2.48792 8 | 1.580084 | N | N | N | 1.4593 8 | 1.96E-05 | 0.219908 | 1.4296 6 | 6.02E-05 | 0.346258 |
| 14 | 24.967 3 | Hydroxyornithine 2 3- | | | 117.8278 | 78.4553 6 | 65.94529 | N | N | N | 1.0691 3 | 0.003448 | 0.559675 | N | N | N |
| 15 | 36.681 | Hydroxypropionic acid 1 3- | 68152 | C01013 | 1.924535 | 19.5080 6 | 10.47345 | N | N | N | 1.4208 8 | 8.67E-06 | 5.442066 | 1.4236 2 | 5.26E-05 | 10.13651 |
| 16 | 12.571 8 | Methylthiopropylamine 4- | | | 17.09075 | 25.0591 9 | 26.06645 | N | N | N | 1.3593 9 | 4.93E-04 | 1.525179 | 1.5159 8 | 7.69E-06 | 1.466243 |
| 17 | 14.099 9 | aminobutyric acid 1 | 12025 | C11118 | 361.931 | 482.818 | 1012.181 | 1.588 44 | 4.63E- 05 | 2.096403 | 1.5310 9 | 5.27E-06 | 2.796614 | 1.1045 5 | 0.002357 | 1.334006 |

| | | | | | | | | | | | | | | | | |
|----|-------------|-------------------------------------|---------|--------|----------|--------------|----------|--------------|--------------|----------|-------------|----------|----------|-------------|----------|----------|
| 18 | 9.2486 9 | 4-aminobutyric acid 3 | 12025 | C11118 | 13.47363 | 19.6908 4 | 41.97504 | 1.609 11 | 3.15E-05 | 2.131704 | 1.5602 4 | 2.75E-06 | 3.115348 | 1.3150 6 | 8.95E-05 | 1.461435 |
| 19 | 9.2966 2 | 4-Androsten-11beta-ol-3,17-dione 1 | | C05284 | 0.55067 | 3.67381 4 | 3.878138 | N | N | N | N | N | N | 1.1995 7 | 0.001032 | 6.671533 |
| 20 | 29.246 | 4-nitrocatechol | 3505109 | C02235 | 6.447669 | 2.27832 1 | 0.299843 | N | N | N | 1.3265 2 | 0.000212 | 0.046504 | N | N | N |
| 21 | 10.445 6 | 4-Vinylphenol dimer | | C05627 | 30.96525 | 67.9696 8 | 67.83964 | N | N | N | 1.3582 7 | 9.58E-05 | 2.190831 | 1.5325 3 | 1.49E-07 | 2.195031 |
| 22 | 14.980 5 | 5-Dihydrocortisol 1 | 164838 | C05471 | 2.285843 | 3.20833 3 | 4.849614 | N | N | N | 1.0697 4 | 0.003736 | 2.121587 | N | N | N |
| 23 | 28.342 7 | Acetol 1 | 164838 | C05471 | 0.073388 | 0.28052 3 | 1.547463 | N | N | N | 1.1165 8 | 0.007093 | 21.08607 | N | N | N |
| 24 | 26.427 1 | Analyte 354 | 8299 | C05235 | 42.92905 | 34.4293 | 27.24397 | 1.011 14 | 0.01613 7 | 0.791302 | 1.1926 6 | 0.000694 | 0.634628 | N | N | N |
| 25 | 27.284 1 | Analyte 368 | | | 6.476845 | 2.2E-05 | 5.013611 | 1.74E +00 | 2.87E-06 | 227592.6 | 1.0177 7 | 6.45E-03 | 0.774082 | 1.6691 5 | 4.31E-08 | 3.4E-06 |
| 26 | 33.476 8 | Analyte 426 | | | 50.41728 | 38.1969 6 | 13.55312 | 1.186 27 | 0.00304 7 | 0.354822 | 1.1317 5 | 0.002547 | 0.268819 | N | N | N |
| 27 | 25.087 7 | Androstanediol | 441301 | C07632 | 0.930614 | 0.69749 7 | 2.159209 | 1.412 44 | 0.00010 4 | 3.095652 | 1.1323 1 | 0.001565 | 2.320197 | N | N | N |
| 28 | 28.307 5 | arbutin | | C06186 | 0.017975 | 0.81600 7 | 2.0204 | 1.225 96 | 0.00237 8 | 2.475961 | 1.6581 6 | 2.74E-08 | 112.401 | 1.0793 4 | 0.00765 | 45.39691 |
| 29 | 20.653 2 | ascorbate | 644104 | C00072 | 4.888771 | 3.22271 2 | 5.9242 | 1.031 16 | 0.01778 9 | 1.838265 | N | N | N | N | N | N |
| 30 | 13.062 2 | asparagine 5 | 6267 | C00152 | 0.237961 | 8.35367 4 | 10.54475 | N | N | N | 1.43560 | 0.000215 | 44.31293 | 1.4088 8 | 0.000171 | 35.10522 |
| 31 | 13.81 | aspartic acid 1 | 83887 | C00402 | 57.56193 | 107.662 3 | 129.8358 | N | N | N | 1.5119 5 | 4.17E-06 | 2.255584 | 1.5768 3 | 1.56E-08 | 1.870374 |
| 32 | 12.561 8 | aspartic acid 2 | | C00049 | 3.153632 | 4.67856 9 | 6.914781 | N | N | N | 1.5257 9 | 2.74E-07 | 2.192641 | N | N | N |
| 33 | 24.002 5 | beta-Mannosylglycerate 1 | | | 12.4809 | 6.61441 1 | 16.58443 | 1.27E +00 | 0.00230 4 | 2.507318 | N | N | N | N | N | N |
| 34 | 28.300 5 | beta-Mannosylglycerate 2 | | | 68.37977 | 80.0231 | 147.6064 | 1.57E +00 | 4.46E-05 | 1.844547 | 1.4997 9 | 5.11E-06 | 2.158626 | N | N | N |
| 35 | 9.6662 9 | Biphenyl Carbobenz | | C06588 | 2.64306 | 0.34606 6 | 6.217126 | 1.624 05 | 3.66E-06 | 17.96517 | 1.1883 4 | 0.001032 | 2.352245 | 1.1741 3 | 0.001064 | 0.130934 |
| 36 | 26.337 7 | xyloxy-L-leucine degr5 | | C04335 | 1.27762 | 2.2E-05 | 0.217431 | N | N | N | 1.3108 7 | 0.000194 | 0.170184 | 1.4319 6 | 0.000132 | 1.72E-05 |
| 37 | 12.253 3 | Carnitine | | C00487 | 2.512566 | 0.96966 5 | 2.485326 | 1.46E +00 | 0.00018 9 | 2.563078 | N | N | N | 1.2655 | 0.000579 | 0.385926 |
| 38 | 13.393 | cis-1,2-Dihydronaphthalene-1,2-diol | | C04314 | 1.41E-05 | 2.2E-05 | 2.893155 | 1.788 26 | 1.10E-07 | 131334.6 | 1.6500 2 | 1.10E-07 | 205263.7 | 1.5143 7 | 1.28E-05 | 1.562907 |
| 39 | 24.682 6 | cis-gondoic acid | 6438157 | | 10.32328 | 12.5970 4 | 5.409907 | 1.057 45 | 0.01452 3 | 0.429459 | N | N | N | N | N | N |
| 40 | 11.220 4 | Citraconic acid degr1 | | | 8.361992 | 10.8744 2 | 11.82222 | N | N | N | N | N | N | 1.3065 9 | 0.000283 | 1.300459 |
| 41 | 18.468 5 | citric acid | 311 | C00158 | 11.37489 | 17.4461 3 | 3.168419 | 1.798 07 | 1.69E-13 | 0.181612 | 1.2859 5 | 0.000455 | 0.278545 | 1.1025 5 | 0.00472 | 1.53374 |
| 42 | 18.661 5 | citrulline 1 | 9750 | C00327 | 17.0663 | 77.7454 7 | 163.7387 | 1.364 68 | 0.00098 6 | 2.106087 | 1.5245 1 | 2.66E-05 | 9.594272 | 1.4891 3 | 1.08E-05 | 4.555496 |
| 43 | 14.616 4 | conduritol b epoxide 1 | | | 1.272426 | 0.69348 | 3.109901 | 1.56E +00 | 6.68E-06 | 4.484487 | 1.3299 9 | 6.94E-05 | 2.444073 | N | N | N |

| | | | | | | | | | | | | | | | | |
|----|-------------|---------------------------------|----------|--------|-----------------|---------------|---------------|-------------|-----------------|-----------------|-------------|----------|----------|-------------|-----------------|-----------------|
| 44 | 15.519 5 | conduititol b epoxide 2 | | | 1.426294 | 0.73504 8 | 0.35044 | 1.13E+00 | 0.00550 2 | 0.476758 | 1.4699 | 1.58E-06 | 0.2457 | 1.2713 9 | 0.000207 | 0.515355 |
| 45 | 20.704 3 | coniferyl alcohol | | C00590 | 1.352264 | 1.00782 7 | 0.440554 | 1.39E+00 | 0.00035 2 | 0.437132 | 1.4551 1 | 5.12E-06 | 0.32579 | N | N | N |
| 46 | 9.0109 3 | cycloleucin e 1 | | C03969 | 20.79575 | 26.5597 | 14.59189 | 1.229 06 | 0.00224 9 | 0.5494 | N | N | N | N | N | N |
| 47 | 17.477 5 | D-(glycerol 1- phosphate) | 439162 | C00093 | 6.601468 | 1.08732 8 | 7.362986 | 1.457 08 | 0.0004 | 6.771631 | N | N | N | 1.6113 | 1.72E-09 | 0.16471 |
| 48 | 25.470 5 | Dehydroep iandroster one | | | 2.548575 | 2.2E-05 | 2.297638 | 1.579 38 | 0.00016 3 | 104301.1 | N | N | N | 1.5255 5 | 1.99E-05 | 8.64E-06 |
| 49 | 20.529 9 | D- erythronol actone 2 | | | 1.171288 | 0.30983 5 | 0.734753 | 1.148 02 | 0.00507 2 | 2.371432 | N | N | N | 1.2001 8 | 0.001171 | 0.264525 |
| 50 | 29.861 4 | D-erythro- sphingosin e 1 | 5262 | C06124 | 3.27121 | 2.64255 8 | 1.687229 | 1.093 87 | 0.00714 4 | 0.638483 | N | N | N | N | N | N |
| 51 | 11.160 4 | D-Glyceric acid | 439194 | C00258 | 7.222751 | 7.83409 4 | 12.39153 | 1.101 28 | 0.01126 7 | 1.581743 | 1.0859 4 | 0.005219 | 1.715624 | N | N | N |
| 52 | 18.921 8 | Diglycerol 2 | | | 27.39385 | 6.58131 5 | 36.72294 | 1.41E+00 | 0.00077 2 | 5.579879 | N | N | N | 1.2166 4 | 0.000966 | 0.240248 |
| 53 | 20.739 | Dihydroxy acetone | 670 | C00184 | 0.014461 | 0.30313 9 | 1.839494 | 1.233 26 | 0.00475 2 | 6.068147 | 1.2846 7 | 0.001831 | 127.1998 | N | N | N |
| 54 | 20.153 3 | D-Talose 2 | | | 47.04185 | 11.4845 2 | 30.96863 | N | N | N | 1.2548 9 | 1.39E-03 | 0.658321 | 1.4751 4 | 2.70E-05 | 0.244134 |
| 55 | 9.5077 9 | epsilon- Caprolacta m | | C06593 | 1.029617 | 3.55728 4 | 0.454674 | 1.695 49 | 1.48E- 08 | 0.127815 | N | N | N | 1.4493 4 | 3.85E-06 | 3.454957 |
| 56 | 10.509 3 | Ethanolam ine | 700 | C00189 | 580.8495 | 455.465 4 | 601.9354 | 1.108 08 | 0.00923 7 | 1.321583 | N | N | N | N | N | N |
| 57 | 12.155 1 | Ethyl cinnamate flavin | 699414 | | 2.026568 | 2.2E-05 | 3.690617 | 1.615 4 | 8.42E- 05 | 167535.3 | N | N | N | 1.3391 7 | 0.000528 | 1.09E-05 |
| 58 | 15.56 | adenine degrad product | | | 2.072325 | 1.71281 7 | 1.220121 | N | N | N | 1.0976 6 | 0.005954 | 0.588769 | N | N | N |
| 59 | 20.788 3 | fructose 1 | 718 | C00354 | 3.296813 | 0.12956 8 | 2.261167 | 1.661 78 | 3.53E- 07 | 17.45154 | N | N | N | 1.0900 7 | 0.006633 | 0.039301 |
| 60 | 17.176 8 | fucose 1 | 439871 | C02985 | 1.729295 | 5.58049 6 | 10.05538 | N | N | N | 1.0207 6 | 0.015125 | 5.814729 | 1.3139 5 | 0.000326 | 3.227035 |
| 61 | 16.648 2 | fucose 2 | 439871 | C02985 | 2.243383 | 3.97562 1 | 7.370288 | 1.021 | 0.02398 5 | 1.853871 | 1.2563 2 | 0.002185 | 3.285345 | 1.1829 5 | 0.001624 | 1.772154 |
| 62 | 11.501 1 | fumaric acid | 723 | C00122 | 15.74363 | 18.7034 7 | 29.09076 | 1.201 19 | 0.00442 4 | 1.555367 | 1.3238 8 | 0.00056 | 1.84778 | N | N | N |
| 63 | 34.593 7 | Galactinol 1 | 439451 | C01236 | 234.7089 | 129.937 3 | 417.118 | 1.64E+00 | 1.69E- 05 | 3.210147 | 1.3079 6 | 1.07E-03 | 1.777171 | 1.5519 2 | 1.56E-07 | 0.553611 |
| 64 | 24.628 4 | Galactinol 3 | 16218555 | | 0.725772 | 0.27292 5 | 1.967361 | 1.639 67 | 2.89E- 07 | 7.208435 | 1.2953 4 | 0.000191 | 2.710716 | N | N | N |
| 65 | 20.415 3 | galactose 2 | 439357 | C00124 | 8.063608 | 2.93133 5 | 4.491522 | N | N | N | N | N | N | 1.0873 2 | 0.004593 | 0.363526 |
| 66 | 19.629 | Gluconic lactone 1 | 7027 | C00198 | 1.41E-05 | 4.01930 7 | 3.213165 | N | N | N | 1.5445 8 | 2.22E-05 | 227967.8 | 1.6149 6 | 1.13E-06 | 285162.1 |
| 67 | 20.782 7 | Gluconic lactone 2 | 7027 | C00198 | 85.46759 | 19.0636 4 | 15.89823 | N | N | N | 1.5779 | 1.86E-08 | 0.186015 | 1.6108 2 | 1.85E-07 | 0.223051 |
| 68 | 20.165 4 | glucose 2 | | C00103 | 5020.921 101 | 9314.54 96 | 6869.253 9 | 1.204 07 | 0.00207 1567 | 0.737475 691 | N | N | N | 1.3125 6 | 9.54939E- 05 | 1.855147 574 |
| 69 | 15.059 4 | Glucose-1- phosphate | | C00103 | 24.15791 | 6.71584 5 | 16.52292 | 1.039 26 | 0.02468 | 2.46029 | N | N | N | N | N | N |
| 70 | 18.894 | glucuronic acid 2 | 439782 | C02670 | 1.445326 | 4.85736 6 | 30.18022 | 1.472 91 | 0.00039 5 | 6.213289 | 1.4293 2 | 0.000166 | 20.88125 | N | N | N |
| 71 | 13.496 7 | glutamine 1 | 5961 | C00064 | 20.61575 | 25.2954 2 | 32.50995 | N | N | N | 1.1772 7 | 0.004458 | 1.576948 | 1.0612 7 | 0.006252 | 1.226995 |

| | | | | | | | | | | | | | | | | |
|-----|-------------|--|---------|--------|----------|--------------|----------|--------------|--------------|----------|-------------|----------|----------|-------------|----------|----------|
| 72 | 13.278 7 | glutamine 3 | 5961 | C00064 | 1.889018 | 1.98646 1 | 15.92764 | 1.000 58 | 0.03074 9 | 8.018095 | N | N | N | N | N | N |
| 73 | 10.427 | glycerol | 753 | C00116 | 167.293 | 287.119 5 | 215.723 | N | N | N | 1.1086 1 | 0.00493 | 1.289492 | N | N | N |
| 74 | 24.955 1 | heptadeca noic acid | 10465 | | 37.63948 | 26.9411 4 | 41.22888 | 1.275 84 | 0.00189 1 | 1.530332 | N | N | N | 1.2535 | 0.000275 | 0.715768 |
| 75 | 19.951 4 | hexadecan e | 10459 | C08260 | 1.41E-05 | 3.18219 4 | 4.643486 | N | N | N | 1.6295 6 | 5.92E-07 | 329446.3 | 1.4132 7 | 0.00018 | 225770.5 |
| 76 | 13.459 8 | indole-3- acetic acid | 802 | C00954 | 0.676482 | 2.2E-05 | 0.480254 | N | N | N | N | N | N | 1.3558 7 | 0.000422 | 3.26E-05 |
| 77 | 24.674 8 | Indolelacta te 2 | 92904 | C02043 | 2.87477 | 12.5970 4 | 6.550944 | 1.181 07 | 0.00607 4 | 0.520038 | N | N | N | 1.3189 9 | 0.00011 | 4.381931 |
| 78 | 21.810 5 | isocitric acid 2 | 5318532 | C00451 | 12.57504 | 4.15245 4 | 4.983046 | N | N | N | 1.1273 2 | 0.002005 | 0.396265 | 1.2836 1 | 0.000856 | 0.330214 |
| 79 | 10.796 3 | Isoleucine | 791 | C00407 | 32.54255 | 30.3937 1 | 84.1354 | 1.64E +00 | 9.19E- 06 | 2.768185 | 1.5192 6 | 2.82E-05 | 2.585397 | N | N | N |
| 80 | 29.185 4 | Isopropyl-beta-D- thiogalactopyranoside | | | 603.3503 | 403.353 3 | 90.85038 | N | N | N | 1.3235 3 | 6.80E-05 | 0.150576 | N | N | N |
| 81 | 8.1024 7 | lactic acid | 107689 | C00186 | 58.3901 | 64.759 | 36.96721 | 1.090 67 | 0.00860 8 | 0.570843 | 1.0696 6 | 0.00403 | 0.633108 | N | N | N |
| 82 | 26.133 9 | Lactobioni c Acid 1 | | | 360.4487 | 518.138 4 | 518.7005 | N | N | N | 1.0358 3 | 0.008524 | 1.439041 | N | N | N |
| 83 | 28.447 6 | lactose 1 | | | 8.016868 | 3.77761 6 | 3.81741 | N | N | N | 1.3623 8 | 2.95E-05 | 0.476172 | 1.1248 4 | 0.002224 | 0.471208 |
| 84 | 11.912 2 | L- Allothreon ine 1 | 99289 | C05519 | 49.14429 | 65.8712 1 | 89.38449 | N | N | N | 1.4008 8 | 0.000103 | 1.818817 | 1.2896 7 | 0.000174 | 1.340363 |
| 85 | 12.630 8 | L-dopa 2 | 836 | C00355 | 1.242659 | 2.45454 2 | 2.699289 | N | N | N | 1.3749 | 2.06E-05 | 2.172187 | 1.151 | 0.001545 | 1.975233 |
| 86 | 24.615 5 | linoleic acid | 3931 | C01595 | 90.54071 | 30.1934 7 | 147.2064 | 1.776 08 | 9.19E- 08 | 4.875438 | 1.4695 5 | 9.50E-05 | 1.625859 | 1.7056 5 | 5.17E-16 | 0.333479 |
| 87 | 23.084 6 | Linoleic acid methyl ester | | | 6.460911 | 5.16735 3 | 16.50972 | 1.037 87 | 0.01423 9 | 3.195006 | 1.002 | 0.018282 | 2.555324 | N | N | N |
| 88 | 24.694 3 | linolenic acid | 860 | C06427 | 15.48884 | 5.15647 8 | 18.97608 | 1.754 96 | 9.40E- 08 | 3.680047 | N | N | N | 1.6928 | 1.39E-14 | 0.332916 |
| 89 | 13.332 7 | L-Malic acid | 222656 | C00149 | 664.732 | 1112.01 6 | 354.7091 | 1.719 65 | 8.33E- 09 | 0.318979 | 1.4804 7 | 2.22E-06 | 0.533612 | 1.4835 1 | 8.33E-06 | 1.672878 |
| 90 | 26.955 5 | L-Threose 1 | 94176 | C03109 | 11.31202 | 4.19343 2 | 5.51266 | N | N | N | N | N | N | 1.0134 2 | 0.011871 | 0.370706 |
| 91 | 15.639 3 | maleic acid | 444266 | C01384 | 4.960352 | 11.0653 5 | 6.367362 | 1.40E +00 | 0.00011 9 | 0.575433 | N | N | N | 1.3561 2 | 4.14E-05 | 2.230758 |
| 92 | 8.6640 5 | Maleimide | | | 2.132515 | 1.17600 7 | 3.981952 | 1.308 44 | 0.00054 7 | 3.385993 | 1.1132 6 | 0.004485 | 1.867256 | N | N | N |
| 93 | 8.3398 8 | malonic acid 1 | | | 18.12768 | 13.9936 6 | 5.337123 | N | N | N | 1.4973 3 | 4.46E-06 | 0.294418 | N | N | N |
| 94 | 13.732 5 | malonic acid 2 | 70615 | | 2.232583 | 0.73927 8 | 0.959232 | N | N | N | 1.1524 7 | 0.001222 | 0.429651 | 1.3598 1 | 0.00028 | 0.331131 |
| 95 | 19.576 7 | mannose 1 | 644175 | C00636 | 2.27604 | 37.0546 2 | 25.10041 | N | N | N | 1.4769 6 | 1.67E-06 | 11.02811 | 1.2477 2 | 0.001035 | 16.2803 |
| 96 | 20.548 3 | methyl heptadeca noate | | | 10.21749 | 1.44364 5 | 12.60037 | 1.728 74 | 3.13E- 06 | 8.728164 | N | N | N | 1.5234 6 | 1.89E-05 | 0.141292 |
| 97 | 20.277 3 | Methyl Palmitoleat e | | | 113.6915 | 121.827 7 | 187.0347 | 1.35E +00 | 0.00084 2 | 1.535239 | 1.2511 1 | 0.000432 | 1.645107 | N | N | N |
| 98 | 9.4139 4 | Methyl Phosphate | 654 | C06608 | 18.46806 | 6.33816 | 10.99532 | N | N | N | 1.1028 1 | 2.26E-03 | 0.59537 | 1.4163 4 | 6.51E-05 | 0.343196 |
| 99 | 10.067 9 | Methylmal onic acid | | | 1.092509 | 1.87989 9 | 2.719165 | N | N | N | 1.39540 | 0.000161 | 2.488917 | 1.1035 1 | 0.004208 | 1.720717 |
| 100 | 31.063 4 | Monoolein | 5280634 | C04230 | 3.150916 | 3.05503 3 | 4.648481 | 1.489 37 | 0.00011 4 | 1.521582 | 1.3307 2 | 0.000206 | 1.475279 | N | N | N |

| | | | | | | | | | | | | | | | | |
|-----|-------------|--|---------|--------|----------|--------------|----------|--------------|--------------|----------|-------------|----------|----------|-------------|----------|----------|
| 101 | 18.313 5 | mucic acid | 3037582 | C01807 | 138.6985 | 146.272 5 | 236.3835 | 1.374 42 | 0.00047 | 1.616049 | 1.3046 2 | 0.000241 | 1.704298 | N | N | N |
| 102 | 23.106 | myo- inositol | 892 | C00137 | 171.5473 | 17.6894 2 | 15.22865 | N | N | N | 1.1045 7 | 0.004441 | 0.088772 | 1.1347 8 | 0.004759 | 0.103117 |
| 103 | 19.450 9 | N-Acetyl- beta-D- mannosam- ine 2 | | | 4.25047 | 8.01696 2 | 150.1214 | 1.543 11 | 0.00016 | 18.72548 | 1.4416 9 | 0.000145 | 35.31879 | N | N | N |
| 104 | 26.387 6 | N- Carbamylg- lutamate 2 | | | 17.611 | 0.49282 7 | 0.342634 | N | N | N | 1.2350 2 | 0.001163 | 0.019456 | 1.2702 8 | 0.001215 | 0.027984 |
| 105 | 9.2802 2 | N-epsilon- Acetyl-L- lysine 2 | 92832 | C02727 | 27.4327 | 44.7570 8 | 58.58672 | N | N | N | 1.3942 9 | 1.36E-05 | 2.135653 | 1.2069 7 | 0.000642 | 1.631523 |
| 106 | 25.873 4 | N-Methyl- L-glutamic acid 3 | | C01046 | 1.912967 | 0.20186 7 | 2.588447 | 1.754 03 | 1.52E- 10 | 12.82253 | N | N | N | 1.6092 9 | 1.76E-09 | 0.105526 |
| 107 | 8.9559 2 | noradrenal- ine | 439260 | C00547 | 34.45356 | 48.1599 5 | 58.963 | N | N | N | 1.3202 4 | 7.43E-04 | 1.711376 | 1.3756 2 | 6.95E-05 | 1.397822 |
| 108 | 9.5245 9 | Norleucine 2 | 21236 | | 3.067261 | 1.99793 2 | 5.760037 | 1.402 15 | 0.00021 9 | 2.882999 | 1.1458 1 | 0.004669 | 1.877909 | N | N | N |
| 109 | 15.268 4 | ornithine | 6262 | C00077 | 1.41E-05 | 4.91811 | 4.270582 | N | N | N | 1.2697 4 | 0.002171 | 302989.5 | 1.2581 7 | 0.001404 | 348930.4 |
| 110 | 13.307 | oxalic acid | 971 | C00209 | 2.28192 | 2.60621 6 | 2.05E-05 | 1.184 56 | 0.00494 9 | 7.88E-06 | 1.4507 5 | 4.58E-05 | 9E-06 | N | N | N |
| 111 | 14.054 3 | oxoproline | 7405 | C01879 | 399.0452 | 329.906 4 | 455.243 | N | N | N | N | N | N | 1.0571 8 | 0.004065 | 0.826739 |
| 112 | 22.368 8 | palmitic acid | 985 | C00249 | 147.4451 | 74.3786 8 | 193.1643 | 1.72E +00 | 3.77E- 07 | 2.597039 | 1.2140 3 | 3.14E-03 | 1.310076 | 1.6618 9 | 1.10E-09 | 0.50445 |
| 113 | 11.722 2 | Pelargonic acid | 8158 | C01601 | 0.974957 | 4.50381 | 3.128425 | N | N | N | N | N | N | 1.0443 6 | 0.010129 | 4.619497 |
| 114 | 23.74 | pentadeca- noic acid | 13849 | | 1.964791 | 0.75046 5 | 2.126913 | 1.74E +00 | 3.50E- 07 | 2.834128 | N | N | N | 1.6371 7 | 4.12E-08 | 0.381957 |
| 115 | 15.646 | phenylalan- ine 1 | | | 9.611323 | 8.91426 7 | 19.23376 | 1.63E +00 | 1.00E- 05 | 2.157637 | 1.4328 2 | 1.44E-05 | 2.001156 | N | N | N |
| 116 | 10.494 | phosphate | 1061 | C00009 | 637.1568 | 299.675 5 | 203.4365 | 1.105 64 | 0.00763 4 | 0.678856 | 1.4449 1 | 9.42E-06 | 0.319288 | 1.3779 1 | 0.000139 | 0.470332 |
| 117 | 10.971 2 | proline | 145742 | C00148 | 1.036378 | 4.22160 4 | 6.495746 | N | N | N | N | N | N | 1.0130 6 | 0.006378 | 4.07342 |
| 118 | 9.9865 5 | Prostaglan- din E2 2 | 5280360 | C00584 | 3.405225 | 0.80885 9 | 3.570587 | 1.586 08 | 3.05E- 06 | 4.414348 | N | N | N | 1.2049 4 | 0.001107 | 0.237535 |
| 119 | 31.966 9 | prunin degr. Prod. 2 | | | 56.36214 | 25.7497 9 | 74.77798 | 1.665 71 | 2.39E- 06 | 2.904023 | N | N | N | 1.5670 2 | 4.64E-08 | 0.456863 |
| 120 | 16.680 2 | ribitol | 827 | C00474 | 2.984962 | 4.38340 5 | 1.193426 | 1.008 91 | 0.01475 7 | 0.27226 | N | N | N | N | N | N |
| 121 | 25.461 1 | ribulose-5- phosphate 2 | 439167 | C00117 | 3.382389 | 1.8884 | 1.883675 | N | N | N | 1.1633 5 | 0.00147 | 0.556907 | 1.3602 2 | 0.000168 | 0.558304 |
| 122 | 32.178 4 | salicin | 439503 | C01451 | 1.681587 | 0.18324 8 | 0.010116 | N | N | N | 1.4020 3 | 0.000114 | 0.006015 | 1.2827 5 | 0.000214 | 0.108973 |
| 123 | 8.5804 1 | sarcosine | 1088 | C00213 | 79.43472 | 112.659 3 | 310.7912 | 1.67E +00 | 1.05E- 05 | 2.758682 | 1.5884 5 | 3.00E-06 | 3.912536 | 1.4237 3 | 9.76E-06 | 1.418263 |
| 124 | 11.569 6 | serine 1 | 106 | C01005 | 32.48561 | 35.8778 1 | 75.87902 | 1.55E +00 | 0.00010 2 | 2.114929 | 1.4480 8 | 3.23E-05 | 2.335774 | N | N | N |
| 125 | 34.206 7 | shikimic acid | 8742 | C00493 | 36.05541 | 28.2023 9 | 13.06826 | 1.456 82 | 0.00017 4 | 0.463374 | N | N | N | N | N | N |
| 126 | 20.308 5 | sorbitol | 5780 | C00794 | 0.201988 | 2.24736 | 2.927416 | N | N | N | 1.2810 1 | 7.47E-04 | 14.49304 | 1.4770 6 | 1.33E-06 | 11.12622 |
| 127 | 31.892 8 | squalene | 1105 | C00751 | 59.9056 | 3.10537 4 | 31.21681 | 1.492 55 | 0.00057 8 | 10.05251 | 1.0784 5 | 3.05E-03 | 0.5211 | 1.5339 7 | 1.60E-05 | 0.051838 |
| 128 | 27.031 5 | stearic acid | 5281 | C01530 | 2.590972 | 0.20358 8 | 3.876497 | 1.72E +00 | 1.62E- 07 | 19.0409 | 1.0129 3 | 7.54E-03 | 1.496156 | 1.5554 6 | 2.64E-07 | 0.078576 |

| | | | | | | | | | | | | | | | | |
|-----|-------------|---|---------|--------|----------|--------------|----------|-------------|--------------|----------|-------------|----------|----------|-------------|----------|----------|
| 129 | 15.723 8 | Tagatose 1 | | | 88.45542 | 48.5220 7 | 59.2265 | N | N | N | 1.3932 4 | 1.64E-05 | 0.669563 | 1.5365 6 | 1.25E-07 | 0.548548 |
| 130 | 27.347 7 | Tagatose 2 | | | 6.535618 | 2.48244 4 | 0.521097 | N | N | N | 1.0349 3 | 0.006992 | 0.079732 | N | N | N |
| 131 | 26.839 2 | Thioctami de 1 | 863 | C00248 | 332.7942 | 174.711 5 | 129.7325 | N | N | N | 1.2000 1 | 0.000754 | 0.389828 | 1.0271 4 | 0.006915 | 0.524984 |
| 132 | 25.178 3 | Threitol | 169019 | | 15.42231 | 14.1495 | 25.4334 | 1.35E+00 | 0.00093 2 | 1.797476 | 1.19860 | 0.002508 | 1.64913 | N | N | N |
| 133 | 14.264 1 | Threonic acid thymidine 5'- monophos phate 1 | 151152 | C01620 | 408.3579 | 1173.13 2 | 353.2065 | 1.68E+00 | 1.42E-06 | 0.30108 | N | N | N | 1.5708 7 | 2.98E-06 | 2.872803 |
| 134 | 24.457 9 | | 9700 | C00364 | 22.08743 | 5.53929 3 | 31.64236 | 1.673 94 | 1.90E-05 | 5.712346 | N | N | N | 1.6592 6 | 1.54E-08 | 0.250789 |
| 135 | 23.280 9 | trans-3,5-Dimethoxy-4- hydroxycinnamaldehyde 1 | | | 1.010234 | 0.52385 4 | 0.109779 | 1.188 53 | 0.00261 1 | 0.209559 | 1.4801 5 | 8.23E-07 | 0.108666 | 1.2029 2 | 0.000617 | 0.518547 |
| 136 | 13.952 6 | trans-4- hydroxy- L-proline 2 | 5810 | C01157 | 0.191149 | 0.57929 2 | 1.363403 | N | N | N | 1.0794 9 | 0.006663 | 7.132678 | N | N | N |
| 137 | 24.363 | Turanose 2 | 5460935 | | 7.318724 | 4.13200 8 | 0.569902 | 1.571 24 | 1.01E-05 | 0.137924 | 1.5236 2 | 1.85E-07 | 0.077869 | 1.2739 1 | 0.000492 | 0.56458 |
| 138 | 20.637 8 | tyrosine 1 | 30819 | C06501 | 32.53049 | 24.1072 8 | 56.6907 | 1.566 97 | 3.39E-05 | 2.351601 | 1.2120 3 | 0.000969 | 1.742694 | N | N | N |
| 139 | 11.416 8 | uracil | 1174 | C00106 | 1.420484 | 3.47286 7 | 6.080578 | 1.25E+00 | 0.00138 3 | 1.750881 | 1.6143 1 | 1.45E-07 | 4.280638 | 1.0946 1 | 0.005904 | 2.444848 |
| 140 | 9.8543 | valine | 1182 | C00183 | 35.56136 | 36.1983 | 118.6639 | 1.707 07 | 2.83E-06 | 3.278163 | 1.5794 3 | 3.20E-06 | 3.336878 | N | N | N |
| 141 | 25.343 1 | xylitol | 6912 | C00379 | 15.66167 | 10.3344 5 | 9.820991 | N | N | N | 1.3774 5 | 2.42E-05 | 0.627072 | 1.3097 6 | 0.000147 | 0.659857 |
| 142 | 27.498 9 | Zymostero 12 | 92746 | C05437 | 86.1823 | 12.5858 5 | 85.45486 | 1.529 67 | 0.00017 4 | 6.789758 | N | N | N | 1.4425 2 | 4.02E-05 | 0.146037 |

Table S3. Changes in the relative content of metabolites related to metabolic pathways in TW, OW and NW.

| RT | Name | KEGG | Relative contents (N) | Relative contents (O) | Relative contents (T) | VIP(T/O) | p-value | FC(T/O) | Log ₂ T/O | VIP(T/N) | p-value | FC (T/N) | Log ₂ T/N | VIP (O/N) | p-value | FC (O/N) | Log ₂ O/N |
|-----------------------|------------------|--------|-----------------------|-----------------------|-----------------------|-------------|--------------|--------------|----------------------|----------|----------|--------------|----------------------|-----------|--------------|--------------|----------------------|
| TCA cycle | | | | | | | | | | | | | | | | | |
| 13.332 7 | L-Malic acid | C00149 | 664.732 | 1112.016 | 354.7091 | 1.7196 5 | 8.33E-09 | 0.31897 9 | - 0.60662 | 1.48047 | 2.22E-06 | 0.53361 2 | - 1.10359 | 1.48351 | 8.33E-06 | 1.67287 8 | 1.347106 |
| 11.501 1 | fumaric acid | C00122 | 15.74363 | 18.70347 | 29.09076 | 1.2011 9 | 0.00442 4 | 1.55536 7 | 1.56923 | 1.32388 | 0.000561 | 1.84778 | 1.12893 2 | N | N | N | 0 |
| 18.468 5 | citric acid | C00158 | 11.37489 | 17.44613 | 3.168419 | 1.7980 7 | 1.69E-13 | 0.18161 2 | - 0.40633 | 1.28595 | 0.000450 | 0.27854 5 | - 0.54229 | 1.10255 | 0.004721 | 1.53374 | 1.620604 |
| 21.810 5 | isocitric acid 2 | C00451 | 12.57504 | 4.152454 | 4.983046 | N | N | N | 0 | 1.12732 | 0.002000 | 0.39626 5 | -0.7488 | 1.28361 | 0.000850 | 0.33021 4 | -0.62558 |
| 15.639 3 | maleic acid | C01384 | 4.960352 | 11.06535 | 6.367362 | 1.40E+00 | 0.00011 9 | 0.57543 3 | - 1.25426 | N | N | N | 0 | 1.35612 | 4.14E-05 | 2.23075 8 | 0.863905 |
| Amino acid metabolism | | | | | | | | | | | | | | | | | |
| 13.81 | aspartic acid 1 | C00402 | 57.56193 | 107.6623 | 129.8358 | N | N | N | 0 | 1.51195 | 4.17E-06 | 2.255580 | 0.85215 1 | 1.57683 | 1.56E-08 | 1.87037 4 | 1.107019 |
| 12.561 8 | aspartic acid 2 | C00049 | 3.153632 | 4.678569 | 6.914781 | N | N | N | 0 | 1.52579 | 2.74E-07 | 2.19264 1 | 0.88287 | N | N | N | 0 |
| 10.796 3 | Isoleucine | C00407 | 32.54255 | 30.39371 | 84.1354 | 1.64E+00 | 9.19E-06 | 2.768180 | 0.68076 3 | 1.51926 | 2.82E-05 | 2.585390 | 0.72972 1 | N | N | N | 0 |
| 9.5245 9 | Norleucin e 2 | | 3.067261 | 1.997932 | 5.760037 | 1.4021 5 | 0.00021 9 | 2.882990 | 0.65463 4 | 1.14581 | 0.004661 | 1.877901 | 0.09995 6 | N | N | N | 0 |
| 10.971 2 | proline | C00148 | 1.036378 | 4.221604 | 6.495746 | N | N | N | 0 | N | N | N | 0 | 1.01306 | 0.00637 8 | 4.07342 | 0.493525 |
| 11.569 6 | serine 1 | C01005 | 32.48561 | 35.87781 | 75.87902 | 1.55E+00 | 0.00010 2 | 2.114920 | 0.92540 4 | 1.44808 | 3.23E-05 | 2.33577 4 | 0.81706 | N | N | N | 0 |

| | | | | | | | | | | | | | | | | | | |
|---|---------------------|--------|----------|----------|----------|----------|----------|-----------------|---------|------------------------|------------------------|-----------------|-----------------|-----------------|-----------------|----------|----------|---|
| 20.6378 | tyrosine 1 | C06501 | 32.53049 | 24.10728 | 56.6907 | 1.56697 | 3.39E-05 | 2.351600.810607 | 1.21203 | 0.000961.742691.247949 | N | N | N | 0 | | | | |
| 9.8543 | valine | C00183 | 35.56136 | 36.1983 | 118.6639 | 1.70707 | 2.83E-06 | 3.278160.583803 | 1.57943 | 3.20E-06 | 3.336870.575208 | N | N | N | 0 | | | |
| Glycolysis | | | | | | | | | | | | | | | | | | |
| 28.3075 | arbutin | C06186 | 0.017975 | 0.816007 | 2.0204 | 1.22596 | 0.002378 | 2.475960.764531 | 1.65816 | 2.74E-08 | 112.4019 | 0.146789 | 1.079340.007651 | 45.39691 | 0.181669 | | | |
| 32.1784 | salicin | C01451 | 1.681587 | 0.183248 | 0.010116 | N | N | N | 0 | 1.40203 | 0.000110.006014 | - | 1.282754 | 0.000210.108973 | -0.3127 | | | |
| 15.0594 | Glucose-1-phosphate | C00103 | 24.15791 | 6.715845 | 16.52292 | 1.03926 | 0.02468 | 2.460295 | 0.76992 | N | N | N | 0 | N | 0 | | | |
| Fructose and mannose metabolism | | | | | | | | | | | | | | | | | | |
| 20.3085 | sorbitol | C00794 | 0.201988 | 2.24736 | 2.927416 | N | N | N | 0 | 1.28101 | 7.47E-04 | 14.49300.259249 | 1.47706 | 1.33E-06 | 11.12622 | 0.287696 | | |
| 19.5767 | mannose 1 | C00636 | 2.27604 | 37.05462 | 25.10041 | N | N | N | 0 | 1.47696 | 1.67E-06 | 11.02810.288751 | 1.247725 | 0.001035 | 16.2803 | 0.248444 | | |
| 20.7883 | fructose 1 | C00354 | 3.296813 | 0.129568 | 2.261167 | 1.66178 | 3.53E-07 | 17.45150.242404 | N | N | N | 0 | 1.090073 | 0.006630.039301 | -0.21417 | | | |
| 17.1768 | fucose 1 | C02985 | 1.729295 | 5.580496 | 10.05538 | N | N | N | 0 | 1.02076 | 0.015125.814720.393745 | 1.313959 | 0.000323.227036 | 0.591643 | | | | |
| 16.6482 | fucose 2 | C02985 | 2.243383 | 3.975621 | 7.370288 | 1.021 | 0.023985 | 1.853871.122913 | 1.25632 | 0.002183.285340.582735 | 1.182955 | 0.001621.772154 | 1.211381 | | | | | |
| Starch and sucrose metablos im | | | | | | | | | | | | | | | | | | |
| 19.9109 | glucose 2 | C00031 | 4315.896 | 152.188 | 2.419958 | N | N | N | 0 | 1.41601 | 8.94E-05 | 0.000561 | -0.0926 | 1.427289 | 9.06E-05 | 0.035262 | -0.20722 | |
| 18.894 | glucuronic acid 2 | C00191 | 1.445326 | 4.857366 | 30.18022 | 1.47291 | 0.000395 | 6.213280.379459 | 1.42932 | 0.0001620.88120.228096 | N | N | N | 0 | | | | |
| Galactose metabolism | | | | | | | | | | | | | | | | | | |
| 34.5937 | Galactinol 1 | C01236 | 234.7089 | 129.9373 | 417.118 | 1.64E+00 | 1.69E-05 | 3.210140.594304 | 1.30796 | 1.07E-03 | 1.777171.205421 | 1.551926 | 1.56E-07 | 0.553611 | -1.17226 | | | |
| 24.6284 | Galactinol 3 | | 0.725772 | 0.272925 | 1.967361 | 1.63967 | 2.89E-07 | 7.208430.350915 | 1.29534 | 0.000192.710710.695081 | N | N | N | 0 | | | | |
| 20.4153 | galactose 2 | C00124 | 8.063608 | 2.931335 | 4.491522 | N | N | N | 0 | N | N | N | 0 | 1.087323 | 0.004590.363526 | -0.68499 | | |
| Pentose and glucuronate interconversions | | | | | | | | | | | | | | | | | | |
| 25.3431 | xylitol | | 15.66167 | 10.33445 | 9.820991 | N | N | N | 0 | 1.37745 | 2.42E-05 | 0.627072 | - | 1.309767 | 0.000140.659857 | -1.66729 | | |
| 16.6802 | ribitol | C00474 | 2.984962 | 4.383405 | 1.193426 | 1.00891 | 0.014757 | 0.27226 | - | N | N | N | 0 | N | N | N | 0 | |
| Phenylalanine, tyrosine and tryptophan biosynthesis | | | | | | | | | | | | | | | | | | |
| 34.2067 | shikimic acid | C00493 | 36.05541 | 28.20239 | 13.06826 | 1.45682 | 0.000174 | 0.463374 | -0.9011 | N | N | N | 0 | N | N | N | 0 | |
| 15.646 | phenylalnine 1 | | 9.611323 | 8.914267 | 19.23376 | 1.63E+00 | 1.00E-05 | 2.157630.901347 | 1.43282 | 1.44E-05 | 2.001150.999166 | N | N | N | 0 | | | |
| Phenylpropanoid biosynthesis | | | | | | | | | | | | | | | | | | |
| 20.7043 | coniferyl alcohol | C00590 | 1.352264 | 1.007827 | 0.440554 | 1.39E+00 | 0.000352 | 0.437132 | - | 1.45511 | 5.12E-06 | 0.32579 | - | 0.61805 | N | N | N | 0 |

Notes: Differential metabolites related to some KEGG pathways were significantly enriched(VIP >1, $p < 0.05$) in TW, OW and NW. T/O represents T vs O, latter are controls, and others are similar.