

Pathway Heat Map This is the heatmap associated with the statistical analysis of the data
Indicates ratios, *p*- and *q*-values for each comparison

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|------|--|
| 0.55 | Green: indicates significant difference ($p \leq 0.05$) between the groups shown; GREEN indicates a metabolite ratio of < 1 |
| 1.71 | Red: indicates significant difference ($p \leq 0.05$) between the groups shown; RED indicates a metabolite ratio of > 1 |
| 1.43 | Bold blue: narrowly missed statistical cutoff for significance; $0.05 < p < 0.10$ |
| 1.20 | Non-colored text and cell: mean values are not significantly different for that comparison |

| Heat map of statistically significant biochemicals profiled in this study. For paired comparisons, shaded cells indicate $p \leq 0.05$ (red indicates that the mean values are significantly higher for that comparison; green values significantly lower). Blue-bolded text indicates $0.05 < p < 0.10$. | | | | | | | | Fold of Change | | | | |
|--|------------------------|---|-------------------------------|-----------|------------------------|-------------------------------|---------------------------|---------------------------|-------------|-------------|-------------|-------------|
| | | | | | | | | Welch's two-Sample T-test | | | | |
| PATHWAY SORT | SUPER PATHWAY | SUB PATHWAY | BIOCHEMICAL NAME | PLATFORM | COMP ID | Kegg | HMDB | Day 0 | Day 5 | | Day 10 | |
| | | | | | | | | | (-CO) | (+CO) | (-CO) | (+CO) |
| 1 | Amino acid | Glycine, serine and threonine metabolism | glycine | GC/MS | 11777 | C00037 | HMDB00123 | 1.06 | 0.65 | 1.23 | 0.71 | 1.01 |
| 3 | | | dimethylglycine | GC/MS | 5086 | C01026 | HMDB00092 | 0.90 | 1.11 | 1.16 | 1.13 | 1.90 |
| 6 | | | beta-hydroxypropyruvate | GC/MS | 15686 | C00168 | HMDB01352 | 1.07 | 0.77 | 1.71 | 1.01 | 1.58 |
| 7 | | | serine | GC/MS | 1648 | C00065 | HMDB03406 | 0.79 | 0.91 | 0.64 | 0.81 | 0.38 |
| 11 | | | homoserine | GC/MS | 23642 | C00263_C02926 | HMDB00719 | 1.14 | 0.82 | 0.74 | 0.82 | 0.38 |
| 16 | | | threonine | GC/MS | 1284 | C00188 | HMDB00167 | 0.61 | 1.04 | 0.76 | 0.72 | 0.52 |
| 23 | | Alanine and aspartate metabolism | alanine | GC/MS | 1126 | C00041 | HMDB00161 | 0.85 | 0.85 | 0.93 | 0.68 | 0.63 |
| 27 | | | N-acetyl-beta-alanine | LC/MS pos | 37432 | C01073 | | 1.09 | 0.93 | 1.14 | 1.14 | 1.48 |
| 29 | | | aspartate | GC/MS | 15996 | C00049 | HMDB00191 | 0.92 | 0.92 | 0.88 | 0.65 | 0.44 |
| 38 | | Glutamate metabolism | glutamate | LC/MS pos | 57 | C00025 | HMDB03339 | 1.13 | 0.90 | 1.17 | 0.91 | 1.28 |
| 41 | | | glutamate, gamma-methyl ester | LC/MS pos | 33487 | | | 1.17 | 0.92 | 1.37 | 0.93 | 1.84 |
| 42 | | | glutamine | GC/MS | 1647 | C00064 | HMDB00641 | 0.95 | 0.79 | 0.76 | 1.89 | 0.33 |
| 44 | | | gamma-aminobutyrate (GABA) | GC/MS | 1416 | C00334 | HMDB00112 | 1.57 | 1.47 | 1.88 | 1.01 | 1.19 |
| 45 | | | N-acetylglutamate | LC/MS pos | 15720 | C00624 | HMDB01138 | 1.10 | 0.89 | 0.94 | 1.07 | 0.43 |
| 48 | | Histidine metabolism | histidine | GC/MS | 59 | C00135 | HMDB00177 | 0.94 | 0.99 | 1.10 | 0.64 | 1.13 |
| 66 | | Lysine metabolism | lysine | LC/MS pos | 1301 | C00047 | HMDB00182 | 0.79 | 1.15 | 0.84 | 0.97 | 0.98 |
| 67 | | | 2-aminoadipate | GC/MS | 6146 | C00956 | HMDB00510 | 1.00 | 1.52 | 1.27 | 0.44 | 0.84 |
| 69 | | | pipecolate | LC/MS pos | 1444 | C00408 | HMDB00070 | 0.90 | 0.95 | 1.51 | 0.58 | 1.66 |
| 74 | | | N6-acetyllysine | LC/MS pos | 36752 | C02727 | HMDB00206 | 0.81 | 1.01 | 1.23 | 0.60 | 1.47 |
| 78 | | Phenylalanine & tyrosine metabolism | phenylalanine | LC/MS pos | 64 | C00079 | HMDB00159 | 0.99 | 1.06 | 1.07 | 0.78 | 1.05 |
| 90 | | | tyrosine | LC/MS pos | 1299 | C00082 | HMDB00158 | 1.00 | 0.96 | 0.97 | 0.65 | 0.70 |
| 126 | | Tryptophan metabolism | tryptophan | LC/MS pos | 54 | C00078 | HMDB00929 | 0.92 | 1.02 | 0.99 | 0.74 | 0.77 |
| 157 | | Valine, leucine and isoleucine metabolism | isoleucine | LC/MS pos | 1125 | C00407 | HMDB00172 | 0.88 | 1.00 | 0.81 | 0.84 | 0.85 |
| 158 | | | leucine | LC/MS pos | 60 | C00123 | HMDB00687 | 0.93 | 0.88 | 0.81 | 0.89 | 0.83 |
| 167 | | | valine | LC/MS pos | 1649 | C00183 | HMDB00883 | 0.93 | 0.91 | 0.74 | 0.83 | 0.48 |
| 188 | | Cysteine, methionine, SAM, taurine metabolism | cysteine | GC/MS | 31453 | C00097 | HMDB00574 | 0.97 | 1.01 | 1.11 | 1.14 | 0.74 |
| 198 | | | adenosylhomocysteine (SAH) | LC/MS pos | 15948 | C00021 | HMDB00939 | 1.22 | 0.98 | 0.87 | 0.83 | 0.68 |
| 213 | | Urea cycle; arginine-, proline-, metabolism | arginine | GC/MS | 1638 | C00062 | HMDB00517 | 0.90 | 0.80 | 0.96 | 0.53 | 0.60 |
| 218 | | | proline | LC/MS pos | 1898 | C00148 | HMDB00162 | 0.97 | 0.72 | 0.83 | 0.72 | 0.46 |
| 220 | | | citulline | LC/MS pos | 2132 | C00327 | HMDB00904 | 1.14 | 0.84 | 0.79 | 0.68 | 0.63 |
| 221 | | | N-acetylmethionine | LC/MS pos | 15630 | C00437 | HMDB03357 | 0.75 | 1.10 | 1.17 | 0.49 | 0.84 |
| 238 | | Polyamine metabolism | 5-methylthioadenosine (MTA) | LC/MS pos | 1419 | C00170 | HMDB01173 | 1.22 | 0.81 | 0.91 | 0.81 | 0.32 |
| 253 | Glutathione metabolism | 5-oxoproline | LC/MS neg | 1494 | C01879 | HMDB00267 | 1.01 | 0.94 | 0.84 | 1.55 | 0.67 | |
| 321 | | gamma-glutamylvaline | LC/MS pos | 32393 | | HMDB11172 | 1.06 | 0.86 | 0.76 | 0.72 | 0.24 | |
| 322 | | gamma-glutamyl-2-aminobutyrate | LC/MS pos | 37092 | | | 0.94 | 1.07 | 0.81 | 1.50 | 0.50 | |
| 323 | | gamma-glutamylleucine | LC/MS pos | 18369 | | HMDB11171 | 1.07 | 0.78 | 0.76 | 0.58 | 0.19 | |
| 324 | | gamma-glutamylisoleucine* | LC/MS pos | 34456 | | HMDB11170 | 1.06 | 0.83 | 0.81 | 0.53 | 0.32 | |
| 327 | | gamma-glutamylmethionine | LC/MS pos | 37539 | | | 1.05 | 1.05 | 0.69 | 0.65 | 0.21 | |

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|-------|--|--|--|---------------------------|---------------------------|---------------------------|-------------------------------------|---------------------------|------|------|------|------|
| 328 | Peptide | gamma-glutamyl | gamma-glutamylglutamate | LC/MS pos | 36738 | | | 0.96 | 0.93 | 1.08 | 0.81 | 0.78 |
| 329 | | | gamma-glutamylglutamine | LC/MS pos | 2730 | | HMDB11738 | 1.03 | 0.85 | 0.65 | 1.26 | 0.23 |
| 331 | | | gamma-glutamylphenylalanine | LC/MS pos | 33422 | | HMDB00594 | 1.10 | 1.00 | 0.80 | 0.58 | 0.41 |
| 332 | | | gamma-glutamyltyrosine | LC/MS pos | 2734 | | | 0.96 | 1.03 | 0.85 | 0.73 | 0.73 |
| 333 | | | gamma-glutamylthreonine* | LC/MS pos | 33364 | | | 1.02 | 0.94 | 0.69 | 0.54 | 0.31 |
| 336 | | | gamma-glutamylalanine | LC/MS pos | 37063 | | | 0.95 | 0.96 | 0.93 | 0.94 | 0.31 |
| 368 | Carbohydrate | Aminosugars metabolism | N-acetylglucosamine | GC/MS | 15095 | C00140 | HMDB00215 | 1.00 | 0.89 | 1.00 | 0.80 | 0.50 |
| 372 | | | erythronate* | GC/MS | 33477 | | HMDB00613 | 1.12 | 0.81 | 1.52 | 1.21 | 2.08 |
| 388 | | Fructose, mannose, galactose, starch, and sucrose metabolism | erythrose | GC/MS | 27722 | C01796 | HMDB02649 | 1.58 | 0.64 | 1.37 | 0.83 | 1.91 |
| 390 | | | galactitol (dulcitol) | GC/MS | 1117 | C01697 | HMDB00107 | 0.88 | 1.44 | 1.02 | 0.71 | 0.57 |
| 391 | | | galactose | GC/MS | 12055 | C01582 | HMDB00143 | 1.18 | 1.00 | 1.00 | 0.36 | 1.00 |
| 397 | | | maltose | GC/MS | 15806 | C00208 | HMDB00163 | 0.97 | 0.70 | 1.01 | 0.67 | 1.12 |
| 402 | | | mannose | GC/MS | 584 | C00159 | HMDB00169 | 0.95 | 0.73 | 1.02 | 0.72 | 0.93 |
| 404 | | | mannose-6-phosphate | GC/MS | 1470 | C00275 | HMDB01078 | 1.00 | 1.29 | 1.02 | 0.93 | 1.18 |
| 410 | | | sorbitol | GC/MS | 15053 | C00794 | HMDB00247 | 0.87 | 1.11 | 1.44 | 1.27 | 1.62 |
| 416 | | | trehalose | GC/MS | 15573 | C01083 | HMDB00975 | 0.97 | 0.88 | 1.02 | 0.59 | 0.69 |
| 432 | | | glycerate | GC/MS | 1572 | C00258 | HMDB00139 | 1.18 | 0.78 | 1.33 | 0.84 | 1.70 |
| 434 | | | Glycolysis, gluconeogenesis, pyruvate metabolism | glucose-6-phosphate (G6P) | GC/MS | 31260 | C00668 | HMDB01401 | 1.06 | 1.19 | 0.87 | 0.92 |
| 436 | | glucose | | GC/MS | 20488 | C00293 | HMDB00122 | 1.17 | 0.93 | 1.25 | 0.99 | 1.85 |
| 439 | | fructose-6-phosphate | | GC/MS | 12021 | C05345 | HMDB00124 | 1.04 | 1.22 | 1.14 | 1.14 | 1.30 |
| 447 | | 1,3-dihydroxyacetone | | GC/MS | 35963 | C00184 | HMDB01882 | 1.07 | 0.78 | 1.36 | 1.03 | 3.05 |
| 457 | | Glyoxylate and dicarboxylate metabolism | | oxalate (ethanedioate) | GC/MS | 20694 | C00209 | HMDB02329 | 1.41 | 0.83 | 1.59 | 0.94 |
| 465 | | Nucleotide sugars, pentose metabolism | sedoheptulose-7-phosphate | GC/MS | 35649 | C05382 | HMDB01068 | 1.33 | 1.23 | 1.18 | 0.90 | 3.55 |
| 466 | | | gluconate | GC/MS | 587 | C00257 | HMDB00625 | 0.78 | 1.16 | 1.28 | 0.78 | 2.01 |
| 468 | ribose | | GC/MS | 12083 | C00121 | HMDB00283 | 1.49 | 1.25 | 0.99 | 0.75 | 0.58 | |
| 475 | Isobar: ribulose 5-phosphate, xylulose 5-phosphate | | GC/MS | 37288 | | | 0.73 | 0.95 | 1.00 | 0.78 | 0.80 | |
| 476 | UDP-glucose | | GC/MS | 32344 | C00029 | HMDB00286 | 1.02 | 0.88 | 1.11 | 0.77 | 0.86 | |
| 480 | arabinose | GC/MS | 575 | C00181 | HMDB00646 | 1.10 | 1.09 | 1.03 | 1.23 | 1.00 | | |
| 491 | Energy | Krebs cycle | citrate | GC/MS | 1564 | C00158 | HMDB00094 | 1.36 | 0.82 | 1.35 | 0.80 | 2.22 |
| 493 | | | cis-aconitate | LC/MS neg | 12025 | C00417 | HMDB00072 | 0.94 | 0.84 | 1.11 | 0.91 | 0.94 |
| 498 | | | isocitrate | LC/MS pos | 12110 | C00311 | HMDB00193.HMDB01874 | 0.98 | 0.94 | 1.50 | 1.06 | 1.82 |
| 500 | | | alpha-ketoglutarate | GC/MS | 33453 | C00026 | HMDB00208 | 1.08 | 1.09 | 1.49 | 0.92 | 1.80 |
| 501 | | | succinate | LC/MS neg | 1437 | C00042 | HMDB00254 | 1.00 | 1.24 | 0.70 | 0.93 | 0.34 |
| 504 | | | fumarate | GC/MS | 1643 | C00122 | HMDB00134 | 1.05 | 0.88 | 1.44 | 0.88 | 1.86 |
| 507 | | malate | GC/MS | 1303 | C00149 | HMDB00156 | 0.80 | 1.27 | 1.58 | 0.75 | 2.66 | |
| 511 | | Oxidative phosphorylation | phosphate | LC/MS neg | 34425 | C00009 | HMDB01429 | 1.00 | 0.97 | 1.00 | 1.01 | 1.09 |
| 512 | | | pyrophosphate (PPi) | GC/MS | 2078 | C00013 | HMDB00250 | 1.14 | 0.62 | 0.94 | 0.44 | 0.68 |
| 512.5 | | Essential fatty acid | linoleate (18:2n6) | linoleate (18:2n6) | LC/MS neg | 1105 | C01595 | HMDB00673 | 0.96 | 1.14 | 1.45 | 1.22 |
| 516 | linolenate [alpha or gamma; (18:3n3 or 6)] | | | LC/MS neg | 34035 | C06427 | HMDB01388 | 1.08 | 1.00 | 1.61 | 1.20 | 6.15 |
| 532 | Medium chain fatty acid | | laurate (12:0) | LC/MS neg | 1645 | C02679 | HMDB00638 | 0.80 | 1.00 | 1.02 | 1.15 | 1.24 |
| 538 | | | palmitate (16:0) | GC/MS | 1336 | C00249 | HMDB00220 | 0.97 | 1.05 | 1.51 | 0.87 | 2.07 |
| 539 | Long chain fatty acid | | palmitoleate (16:1n7) | GC/MS | 1507 | C08362 | HMDB03229 | 1.27 | 0.54 | 1.69 | 1.32 | 4.69 |
| 541 | | | margarate (17:0) | LC/MS neg | 1121 | | HMDB02259 | 0.89 | 0.91 | 1.22 | 1.07 | 1.54 |
| 542 | | | 10-heptadecenoate (17:1n7) | LC/MS neg | 33971 | | | 0.95 | 0.92 | 1.42 | 1.14 | 4.03 |
| 543 | | | stearate (18:0) | GC/MS | 1358 | C01530 | HMDB00827 | 0.87 | 1.11 | 1.17 | 1.00 | 1.49 |
| 544 | | | tuberculostearate | GC/MS | 34163 | | HMDB04085 | 1.05 | 0.98 | 1.16 | 1.18 | 0.86 |
| 545 | | | oleate (18:1n9) | LC/MS neg | 1359 | C00712 | HMDB00207 | 1.03 | 1.21 | 1.30 | 1.18 | 6.42 |

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|-------|---|---|-----------|-------|-------------------------------|-------------------------------------|------|------|------|------|-------|
| 554 | | 10-nonadecenoate (19:1n9) | LC/MS neg | 33972 | | | 1.23 | 1.00 | 1.07 | 0.99 | 8.63 |
| 573 | | lignocerate (24:0) | GC/MS | 1364 | C08320 | HMDB02003 | 1.00 | 1.00 | 1.23 | 1.00 | 3.49 |
| 576 | | hexacosanoate (26:0) | GC/MS | 21143 | | HMDB02356 | 1.01 | 1.12 | 1.29 | 1.00 | 3.90 |
| 589 | Fatty acid, ester | n-Butyl Oleate | GC/MS | 36802 | | | 0.99 | 1.04 | 0.91 | 0.80 | 1.28 |
| 591 | | 4-hydroxybutyrate (GHB) | GC/MS | 34585 | C00989 | HMDB00710 | 1.00 | 1.04 | 0.90 | 1.08 | 1.80 |
| 596 | | 8-hydroxyoctanoate | LC/MS neg | 21239 | | HMDB00711 | 1.13 | 0.87 | 0.81 | 1.13 | 1.78 |
| 599 | Fatty acid, monohydroxy | 2-hydroxymyristate | LC/MS neg | 32413 | C13790 | HMDB02261 | 0.82 | 1.18 | 1.00 | 1.12 | 1.27 |
| 602 | | 2-hydroxystearate | LC/MS neg | 17945 | C03045 | | 1.02 | 1.24 | 1.01 | 0.86 | 1.05 |
| 604 | | 2-hydroxypalmitate | LC/MS neg | 35675 | | | 0.93 | 1.02 | 0.83 | 1.13 | 1.51 |
| 608 | | 13-HODE + 9-HODE | LC/MS neg | 37752 | | | 2.81 | 3.31 | 1.91 | 0.77 | 12.18 |
| 615 | Fatty acid, dicarboxylate | sebacate (decanedioate) | LC/MS neg | 32398 | C08277 | HMDB00792 | 1.02 | 1.06 | 1.13 | 1.08 | 1.58 |
| 616 | | azelate (nonanedioate) | LC/MS neg | 18362 | C08261 | HMDB00784 | 0.81 | 1.24 | 1.00 | 1.21 | 1.37 |
| 619 | | hexadecanedioate | LC/MS neg | 35678 | | HMDB00672 | 0.86 | 0.77 | 1.15 | 1.24 | 1.88 |
| 626 | Fatty acid, amide | stearamide | LC/MS pos | 37487 | C13846 | | 0.97 | 1.04 | 0.85 | 1.37 | 1.20 |
| 632.6 | Fatty acid, branched | 15-methylpalmitate | GC/MS | 38295 | | | 1.00 | 1.82 | 1.88 | 0.66 | 7.46 |
| 679 | Endocannabinoid | palmitoylethanolamide | LC/MS neg | 38165 | | | 0.95 | 0.86 | 1.15 | 1.13 | 1.07 |
| 679.1 | | stearoylethanolamide | GC/MS | 38625 | | | 1.03 | 0.97 | 1.22 | 0.87 | 0.95 |
| 744 | Fatty alcohol, long chain | 1-octadecanol | GC/MS | 21128 | D01924 | HMDB02350 | 0.60 | 0.84 | 1.87 | 1.21 | 1.76 |
| 746 | | ethanolamine | GC/MS | 34285 | C00189 | HMDB00149 | 0.91 | 0.89 | 1.29 | 0.91 | 1.10 |
| 749 | | diethanolamine | GC/MS | 20691 | C06772 | HMDB04437 | 0.83 | 1.05 | 0.96 | 0.92 | 1.12 |
| 750 | Glycerolipid metabolism | glycerol | GC/MS | 15122 | C00116 | HMDB00131 | 1.06 | 0.83 | 1.24 | 0.76 | 1.66 |
| 752 | | glycerol 3-phosphate (G3P) | GC/MS | 15365 | C00093 | HMDB00126 | 1.02 | 0.69 | 0.70 | 0.96 | 0.14 |
| 760 | Inositol metabolism | myo-inositol | GC/MS | 19934 | C00137 | HMDB00211 | 0.98 | 1.00 | 0.69 | 0.88 | 0.32 |
| 763 | | inositol 1-phosphate (I1P) | GC/MS | 1481 | | HMDB00213 | 0.94 | 0.80 | 1.03 | 1.01 | 0.40 |
| 776 | Lysolipid | 2-palmitoylglycerophosphoethanolamine* | LC/MS pos | 35684 | | | 0.96 | 0.79 | 0.60 | 0.92 | 0.28 |
| 813 | | 1-docosahexaenoylglycerophosphocholine* | LC/MS pos | 33822 | | | 2.13 | 1.00 | 1.89 | 1.14 | 0.46 |
| 955 | | adenine | GC/MS | 554 | C00147 | HMDB00034 | 1.22 | 0.61 | 0.71 | 0.82 | 0.25 |
| 956 | | adenosine | LC/MS pos | 555 | C00212 | HMDB00050 | 1.18 | 0.98 | 1.13 | 0.72 | 0.69 |
| 964 | | adenosine 5'-monophosphate (AMP) | LC/MS pos | 32342 | C00020 | HMDB00045 | 1.07 | 0.89 | 0.83 | 0.92 | 0.27 |
| 966.5 | Purine metabolism, adenine containing | adenosine-5'-diphosphoglucose | LC/MS neg | 35652 | C06192,C00498 | HMDB06369.HMDB06557 | 0.92 | 0.72 | 0.99 | 0.84 | 0.36 |
| 970 | Nucleotide | adenosine 3',5'-cyclic monophosphate (cAMP) | LC/MS neg | 2831 | C00575 | HMDB00058 | 0.83 | 0.72 | 0.91 | 0.52 | 1.60 |
| 1016 | Pyrimidine metabolism, thymine containing | thymine | GC/MS | 604 | C00178 | HMDB00262 | 1.07 | 0.94 | 0.78 | 0.88 | 0.51 |
| 1019 | | thymidine 5'-monophosphate | LC/MS neg | 12023 | C00364 | HMDB01227 | 1.14 | 0.83 | 0.75 | 1.24 | 0.41 |
| 1022 | Pyrimidine metabolism, uracil containing | uracil | GC/MS | 605 | C00106 | HMDB00300 | 0.91 | 0.61 | 0.74 | 0.75 | 1.26 |
| 1036 | Purine and pyrimidine metabolism | methylphosphate | GC/MS | 37070 | | | 0.99 | 0.84 | 1.02 | 1.08 | 1.15 |
| 1047 | Biotin metabolism | biotin | LC/MS pos | 568 | C00120 | HMDB00030 | 1.24 | 0.91 | 1.36 | 0.97 | 2.01 |
| 1063 | | nicotinamide | LC/MS pos | 594 | C00153 | HMDB01406 | 0.96 | 0.82 | 1.23 | 0.77 | 1.34 |
| 1066 | Nicotinate and nicotinamide metabolism | nicotinamide adenine dinucleotide (NAD+) | LC/MS pos | 5278 | C00003 | HMDB00902 | 0.97 | 0.76 | 0.63 | 1.03 | 0.14 |
| 1077 | | nicotinate | LC/MS pos | 1504 | C00253 | HMDB01488 | 1.26 | 0.83 | 1.21 | 0.92 | 0.60 |
| 1079 | Cofactors and vitamins | nicotinic acid mononucleotide (NaMN) | LC/MS pos | 32461 | | HMDB01132 | 1.27 | 1.09 | 0.73 | 1.11 | 0.77 |
| 1080 | | nicotinate ribonucleoside* | LC/MS pos | 33471 | C05841 | HMDB06809 | 1.17 | 1.08 | 0.90 | 0.98 | 0.83 |

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|--------|---------------------------------|----------------------------|-------------------------|-----------|-------------------------------|---------------------------|---------------------------|-------------|-------------|-------------|-------------|
| 1085 | Pantothenate and CoA metabolism | pantothenate | LC/MS pos | 1508 | C00864 | HMDB00210 | 0.94 | 1.07 | 0.70 | 1.25 | 0.54 |
| 1089 | | acetyl CoA | LC/MS neg | 32484 | C00024 | HMDB01206 | 1.06 | 1.20 | 1.18 | 1.06 | 0.63 |
| 1119 | | Vitamin B6 metabolism | pyridoxine (Vitamin B6) | LC/MS pos | 608 | C00314 | HMDB02075 | 1.17 | 0.92 | 1.31 | 0.94 |
| 1128 | Benzoate metabolism | 2-(hydroxymethyl)phenol | GC/MS | 37492 | C02323 | | 1.40 | 0.77 | 0.97 | 0.67 | 1.20 |
| 1137 | | 4-hydroxybenzoate | GC/MS | 21133 | C00156 | HMDB00500 | 1.08 | 0.98 | 0.95 | 0.86 | 0.86 |
| 1150 | Chemical | bicine | GC/MS | 20708 | | HMDB11727 | 0.87 | 1.18 | 0.96 | 0.90 | 1.19 |
| 1151 | | glycolate (hydroxyacetate) | GC/MS | 15737 | C00160 | HMDB00115 | 1.08 | 0.90 | 1.29 | 1.06 | 1.61 |
| 1157 | | glycerol 2-phosphate | GC/MS | 27728 | C02979_D01488 | HMDB02520 | 1.08 | 0.66 | 0.80 | 0.84 | 0.55 |
| 1161 | | heptaethylene glycol | LC/MS pos | 38154 | | | 1.21 | 0.98 | 1.39 | 0.96 | 2.08 |
| 1162 | | hexaethylene glycol | LC/MS pos | 38133 | | | 1.19 | 0.93 | 1.62 | 0.92 | 2.22 |
| 1165 | | tetraethylene glycol | LC/MS pos | 38101 | | | 0.96 | 0.65 | 1.65 | 1.02 | 1.94 |
| 1165.5 | | diethylene glycol | GC/MS | 38099 | | | 2.50 | 0.77 | 1.06 | 0.74 | 1.47 |
| 1175 | | trizma acetate | GC/MS | 20710 | C07182 | | 0.11 | 0.41 | 1.32 | 0.39 | 0.56 |
| 1196.5 | | cyclohexylamine* | GC/MS | 33452 | C00571 | | 1.09 | 1.17 | 1.10 | 0.94 | 1.25 |
| 1206.6 | | dexpanthenol | LC/MS pos | 38314 | D03726 | HMDB04231 | 0.86 | 0.80 | 0.98 | 0.68 | 0.29 |
| 1207.9 | | 3-(2-pyrrolidinyl)pyridine | LC/MS pos | 38122 | | | 1.08 | 1.08 | 1.21 | 1.04 | 1.31 |
| 1212 | Drug | salicylate | GC/MS | 1515 | C00805 | HMDB01895 | 0.81 | 0.85 | 1.91 | 0.87 | 0.92 |
| 1287 | Food component/Plant | 4-hydroxybenzyl alcohol | GC/MS | 15127 | C17467 | HMDB11724 | 22.52 | 0.91 | 0.89 | 0.55 | 1.02 |
| 1330 | | ergothioneine | LC/MS pos | 37459 | C05570 | HMDB03045 | 1.02 | 0.81 | 0.49 | 0.98 | 0.11 |
| 1334 | | 5-hydroxymethylfurfural | LC/MS pos | 37429 | C11101 | | 1.77 | 0.79 | 1.19 | 1.41 | 2.25 |
| 1358 | Sugar, sugar substitute, starch | trehalose 6-phosphate | GC/MS | 15802 | C00689 | HMDB01124 | 1.00 | 0.69 | 0.53 | 0.56 | 0.24 |
| 1360 | | erythritol | GC/MS | 20699 | C00503 | HMDB02994 | 1.20 | 0.81 | 1.43 | 0.82 | 1.47 |
| 1380.1 | Bacterial | mycothione (MSSM)* | LC/MS pos | 38682 | | | 0.99 | 0.83 | 0.57 | 0.85 | 0.12 |