|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Supplementary Table S5 - Raw metabolomics data | | |  |  |  |  |  |  |
| **CONTROLS -** | **T0** | | | | | |  |  |
| **sample name** | Sample\_1 | Sample\_2 | Sample\_3 | Sample\_4 | Sample\_5 | Sample\_6 | **Average** |  |
| 1-Methyladenosine | 0.0157 | 0.0142 | 0.0125 | 0.0076 | 0.0056 | 0.011 | **0.0111** |  |
| 1-Methylhistidine | 0.0157 | 0.0099 | 0.0104 | 0.0062 | 0.0182 | 0.0073 | **0.01128333** |  |
| 2-Aminooctanoic acid | 0.007 | 0.0059 | 0.0086 | 0.0122 | 0.003 | 0.0165 | **0.00886667** |  |
| 2-Furoic acid | 0.4966 | 0.0774 | 0.5875 | 0.1891 | 0.2854 | 0.243 | **0.31316667** |  |
| 2-Isopropylmalic acid | 0.0066 | 0.004 | 0.0049 | 0.0044 | 0.008 | 0.0075 | **0.0059** |  |
| 2-Methyl-3-ketovaleric acid | 0.2456 | 0.3185 | 0.2172 | 0.183 | 0.3526 | 0.41 | **0.28781667** |  |
| 2-Methylglutaric acid | 0.0073 | 0.0098 | 0.0082 | 0.0022 | 0.0058 | 0.0051 | **0.0064** |  |
| 2-Piperidinone | 0.0103 | 0.0099 | 0.0088 | 0.0058 | 0.0016 | 0.0091 | **0.00758333** |  |
| 2-Pyrrolidinone | 0.0009 | 0.0027 | 0.001 | 0.0007 | 0.0015 | 0.0011 | **0.00131667** |  |
| 3-Indolepropionic acid | 0.0022 | 0.0026 | 0.0018 | 0 | 0 | 0 | **0.0011** |  |
| 3-Methoxybenzenepropanoic acid | 0.005 | 0.0043 | 0.0034 | 0.003 | 0.0026 | 0.0057 | **0.004** |  |
| 3-Methylindole | 0.041 | 0.0239 | 0.0377 | 0.0326 | 0.0768 | 0.0739 | **0.04765** |  |
| 5-Hydroxyindoleacetic acid | 0.0801 | 0.0559 | 0.0191 | 0.0079 | 0.0053 | 0.0046 | **0.02881667** |  |
| 7-Methylguanine | 0.0226 | 0.0183 | 0.0221 | 0.0127 | 0.0173 | 0.022 | **0.01916667** |  |
| Acetylglycine | 0.0032 | 0.005 | 0.0021 | 0.0015 | 0.0012 | 0 | **0.00216667** |  |
| Allantoin | 0.1264 | 0.0857 | 0.1094 | 0.0533 | 0.101 | 0.0407 | **0.08608333** |  |
| Ascorbic acid | 0.0341 | 0.0376 | 0.0317 | 0.0246 | 0.0276 | 0.0456 | **0.03353333** |  |
| Asymmetric dimethylarginine and Symmetric dimethylarginine | 0.0879 | 0.0841 | 0.0866 | 0.0482 | 0.074 | 0.1027 | **0.08058333** |  |
| Azelaic acid | 0.1908 | 0.195 | 0.1932 | 0.1055 | 0.1091 | 0.1966 | **0.16503333** |  |
| Betaine | 1.4731 | 1.2804 | 1.1951 | 0.5866 | 1.3366 | 1.0227 | **1.14908333** |  |
| Butyric acid | 0 | 0 | 0 | 0 | 0.0021 | 0.0038 | **0.00098333** |  |
| C10H19N3O5 | 0.0196 | 0.0165 | 0.0185 | 0.0101 | 0.011 | 0.0281 | **0.0173** |  |
| C10H7NO2 | 0.0137 | 0.0039 | 0.0136 | 0.0032 | 0.0023 | 0.0028 | **0.00658333** |  |
| C10H9NO3 | 0.0431 | 0.0137 | 0.0471 | 0.0094 | 0.0047 | 0.007 | **0.02083333** |  |
| C11H19NO9 | 0.0038 | 0.0027 | 0.0024 | 0.0033 | 0.0057 | 0.0472 | **0.01085** |  |
| C18H39NO2 | 0.083 | 0.1079 | 0.1522 | 0.002 | 0.0029 | 0.0045 | **0.05875** |  |
| C24H38O5 | 0.0041 | 0.02 | 0.0018 | 0.0017 | 0.0007 | 0.1353 | **0.02726667** |  |
| C33H36N4O6 | 0.0148 | 0.0365 | 0 | 0.0178 | 0.0209 | 0.0261 | **0.01935** |  |
| C5H10O5 | 0.0477 | 0.0216 | 0.0294 | 0.0091 | 0.0128 | 0.0103 | **0.02181667** |  |
| C6H10O6 | 0.0297 | 0.034 | 0.0289 | 0.0222 | 0.0267 | 0.039 | **0.03008333** |  |
| C6H8N2O2 | 0.0117 | 0.0084 | 0.0111 | 0.0059 | 0.0192 | 0.0069 | **0.01053333** |  |
| C6H8O4 | 0.0046 | 0.0089 | 0.006 | 0.0018 | 0.0051 | 0.0016 | **0.00466667** |  |
| C9H10N2O5 | 0.0116 | 0.0023 | 0.0042 | 0.0005 | 0 | 0 | **0.0031** |  |
| C9H13NO | 0.0913 | 0.0566 | 0.0999 | 0.0265 | 0.1104 | 0.0768 | **0.07691667** |  |
| C9H13NO3 | 0.002 | 0.0034 | 0.0019 | 0.0006 | 0.0012 | 0.0023 | **0.0019** |  |
| C9H6O2 | 0.0458 | 0.0556 | 0.0464 | 0.0202 | 0.0708 | 0.0871 | **0.05431667** |  |
| C9H9NO4 | 0.0096 | 0.0105 | 0.0079 | 0.0134 | 0.0641 | 0.041 | **0.02441667** |  |
| Carvone | 0.0267 | 0.0186 | 0.0255 | 0.0085 | 0.0166 | 0.0264 | **0.02038333** |  |
| Cholic acid | 0.0625 | 1.5555 | 0.15 | 0.0771 | 0.0175 | 0.2811 | **0.35728333** |  |
| Choline | 0.0996 | 0.1043 | 0.0966 | 0.0601 | 0.0868 | 0.1643 | **0.10195** |  |
| Cinnamic acid | 0.1948 | 0.2897 | 0.1957 | 0.1183 | 0.1714 | 0.2456 | **0.20258333** |  |
| Citric acid | 1.7941 | 0.2911 | 2.029 | 0.6582 | 0.9952 | 0.8298 | **1.09956667** |  |
| Citrulline | 0.0157 | 0.0124 | 0.0161 | 0.0177 | 0.0151 | 0.0349 | **0.01865** |  |
| Creatine | 1.0544 | 0.8918 | 1.2121 | 1.1184 | 0.7999 | 1.3241 | **1.06678333** |  |
| Creatinine | 0.2849 | 0.2037 | 0.2465 | 0.1513 | 0.2594 | 0.2561 | **0.23365** |  |
| Cytosine | 0.1293 | 0.1055 | 0.0501 | 0.1009 | 0.091 | 0.0636 | **0.09006667** |  |
| Deoxycytidine | 0.007 | 0.0092 | 0.0021 | 0.0034 | 0.0135 | 0.0024 | **0.00626667** |  |
| Desaminotyrosine | 0.0151 | 0.0211 | 0.0332 | 0.0239 | 0.1154 | 0.0469 | **0.0426** |  |
| Dimethyl sulfone | 0.0019 | 0.0027 | 0.0029 | 0.001 | 0.0006 | 0.0018 | **0.00181667** |  |
| Dimethylmalonic acid | 0.0085 | 0.0049 | 0.0066 | 0.0039 | 0.0065 | 0.0109 | **0.00688333** |  |
| Disaccaride - C12H22O11 | 0.0276 | 0.0326 | 0.0296 | 0.0122 | 0.0137 | 0.0188 | **0.02241667** |  |
| Fumaric acid | 0.0079 | 0.008 | 0.008 | 0.0043 | 0.0105 | 0.0104 | **0.00818333** |  |
| Galacturonic acid | 0.0414 | 0.045 | 0.0423 | 0.0296 | 0.0357 | 0.0503 | **0.04071667** |  |
| Gluconic acid | 0.05 | 0.0574 | 0.0609 | 0.0358 | 0.0873 | 0.0559 | **0.05788333** |  |
| Glycerophosphocholine | 0.0269 | 0.0159 | 0.0275 | 0.0166 | 0.02 | 0.0408 | **0.02461667** |  |
| Glycocholic acid | 1.6315 | 1.2942 | 1.5033 | 0.874 | 0.2108 | 2.9606 | **1.4124** |  |
| Hippuric acid | 0.2778 | 0.1644 | 0.1771 | 0.0656 | 0.0645 | 0.1761 | **0.15425** |  |
| Homocitrulline | 0.0054 | 0.0029 | 0.0043 | 0.0026 | 0.0099 | 0.0034 | **0.00475** |  |
| Hydroxyisobutyric acid | 0.0505 | 0.0704 | 0.0385 | 0.0535 | 0.0859 | 0.1027 | **0.06691667** |  |
| Hydroxyphenyllactic acid | 0.0874 | 0.1361 | 0.1033 | 0.052 | 0.4286 | 0.1859 | **0.16555** |  |
| Hypoxantine | 0.002 | 0.0019 | 0.0018 | 0.0011 | 0.0018 | 0.0039 | **0.00208333** |  |
| Indoleacetic acid | 0.0042 | 0.0008 | 0.0071 | 0.0019 | 0.0038 | 0.0026 | **0.0034** |  |
| Indoleacrylic acid | 1.3852 | 0.8333 | 1.2923 | 1.059 | 2.729 | 2.5331 | **1.63865** |  |
| Indolelactic acid | 0.2326 | 0.1415 | 0.2366 | 0.1269 | 1.1312 | 0.2054 | **0.3457** |  |
| Kynurenine | 0.0717 | 0.0165 | 0.0662 | 0.015 | 0.0109 | 0.0134 | **0.03228333** |  |
| L-Acetylcarnitine | 0.1565 | 0.3105 | 0.2155 | 0.0882 | 0.3011 | 0.0781 | **0.19165** |  |
| Lactic acid | 0.6195 | 0.5119 | 0.4457 | 0.4417 | 0.9267 | 0.7913 | **0.6228** |  |
| L-Alanine | 0.0089 | 0.0075 | 0.0108 | 0.009 | 0.0078 | 0.0117 | **0.00928333** |  |
| L-Arginine | 0.3274 | 0.3277 | 0.2657 | 0.2398 | 0.1106 | 0.5461 | **0.30288333** |  |
| L-Carnitine | 0.121 | 0.1817 | 0.2166 | 0.0757 | 0.2244 | 0.0927 | **0.15201667** |  |
| L-Glutamic acid | 0.0351 | 0.0454 | 0.0405 | 0.0233 | 0.0963 | 0.0968 | **0.05623333** |  |
| L-Glutamine | 0.0163 | 0.018 | 0.0169 | 0.0066 | 0 | 0.0036 | **0.01023333** |  |
| L-Histidine | 0.0287 | 0.0293 | 0.0338 | 0.0333 | 0.0456 | 0.1048 | **0.04591667** |  |
| L-Leucine + L-Isoleucine | 0.7206 | 0.7062 | 0.5634 | 0.4424 | 0.5711 | 1.246 | **0.70828333** |  |
| L-Lysine | 0.0094 | 0.0086 | 0.0071 | 0.0043 | 0.0062 | 0.0121 | **0.00795** |  |
| L-Methionine | 0.1123 | 0.1152 | 0.1103 | 0.0897 | 0.1823 | 0.3007 | **0.15175** |  |
| L-Phenylalanine | 0.652 | 0.8583 | 0.6222 | 0.3705 | 0.6204 | 0.881 | **0.6674** |  |
| L-Proline | 0.3873 | 0.3388 | 0.3774 | 0.2214 | 0.6723 | 0.981 | **0.49636667** |  |
| L-Threonine | 0.0057 | 0.004 | 0.0065 | 0.0036 | 0.0055 | 0.008 | **0.00555** |  |
| L-Tryptophan | 0.315 | 0.1768 | 0.285 | 0.2336 | 0.6235 | 0.5282 | **0.36035** |  |
| L-Tyrosine | 0.2222 | 0.2793 | 0.2392 | 0.1011 | 0.3596 | 0.4279 | **0.27155** |  |
| L-Valine | 0.2174 | 0.2094 | 0.178 | 0.1565 | 0.209 | 0.4207 | **0.23183333** |  |
| Malic acid | 0.0288 | 0.028 | 0.0288 | 0.0168 | 0.0391 | 0.0362 | **0.02961667** |  |
| Mesaconic acid | 0.0227 | 0.0403 | 0.0335 | 0.0129 | 0.0165 | 0.0171 | **0.02383333** |  |
| Monosaccaride - C6H12O6 | 0.2632 | 0.0978 | 0.0718 | 0.0577 | 0.0814 | 0.0932 | **0.11085** |  |
| N-Acetyl-L-phenylalanine | 0.0209 | 0.0088 | 0.0041 | 0.012 | 0.0176 | 0.0146 | **0.013** |  |
| Niacinamide | 0.3817 | 0.3706 | 0.4864 | 0.4366 | 0.0286 | 0.0196 | **0.28725** |  |
| Nutriacholic acid | 0.0094 | 0.0292 | 0.011 | 0.0046 | 0.014 | 0.0129 | **0.01351667** |  |
| Ornithine | 0.0775 | 0.0623 | 0.0683 | 0.0688 | 0.0459 | 0.1101 | **0.07215** |  |
| Oxoglutaric acid | 0.0726 | 0.0836 | 0.0608 | 0.0797 | 0.3221 | 0.259 | **0.1463** |  |
| Pantothenic acid | 0.0657 | 0.0529 | 0.0647 | 0.0484 | 0.1161 | 0.0887 | **0.07275** |  |
| Phenylacetaldehyde | 0.0154 | 0.0226 | 0.0181 | 0.0081 | 0.0278 | 0.0347 | **0.02111667** |  |
| Phenylacetylglycine | 0.3392 | 0.1003 | 0.3422 | 0.0356 | 0.0127 | 0.0387 | **0.14478333** |  |
| Pipecolic acid | 0.0363 | 0.0213 | 0.0307 | 0.0177 | 0.0291 | 0.0268 | **0.02698333** |  |
| Pyroglutamic acid | 0.1404 | 0.1517 | 0.1475 | 0.0803 | 0.1318 | 0.1974 | **0.14151667** |  |
| Riboflavin | 0.0142 | 0.008 | 0.009 | 0.0042 | 0.011 | 0.0054 | **0.00863333** |  |
| Ribothymidine | 0.0296 | 0.0326 | 0.0561 | 0.0259 | 0.0076 | 0.0355 | **0.03121667** |  |
| Sebacic acid | 0.0665 | 0.0772 | 0.0693 | 0.0427 | 0.0661 | 0.0869 | **0.06811667** |  |
| Suberic acid | 0.0404 | 0.0341 | 0.038 | 0.0275 | 0.0381 | 0.0593 | **0.03956667** |  |
| Succinic acid | 0.0278 | 0.027 | 0.0217 | 0.0192 | 0.0438 | 0.08 | **0.03658333** |  |
| Succinic acid semialdehyde | 0.0124 | 0.0123 | 0.0097 | 0.0121 | 0.048 | 0.0397 | **0.02236667** |  |
| Taurine | 0.0512 | 0.0537 | 0.0536 | 0.0214 | 0.0534 | 0.0143 | **0.04126667** |  |
| Taurocholic acid | 0.4352 | 0.313 | 0.3009 | 0.1994 | 0.0975 | 0.8638 | **0.3683** |  |
| Taurodeoxycholic acid | 0.1455 | 0.0922 | 0.1077 | 0.0441 | 0.1135 | 0.196 | **0.1165** |  |
| Thymidine | 0.1413 | 0.2958 | 0.2168 | 0.0791 | 0.5573 | 0.0536 | **0.22398333** |  |
| Thymine | 0.0255 | 0.0389 | 0.0298 | 0.0178 | 0.0918 | 0.0206 | **0.0374** |  |
| Traumatic acid | 0.0224 | 0.0244 | 0.0197 | 0.031 | 0.0717 | 0.0458 | **0.03583333** |  |
| Uracil | 0.028 | 0.0217 | 0.0475 | 0.0241 | 0.0004 | 0.0042 | **0.02098333** |  |
| Uric Acid | 0.6446 | 0.5067 | 0.4911 | 0.1794 | 0.3096 | 0.255 | **0.39773333** |  |
| Uridine | 0.0046 | 0.0036 | 0.0109 | 0.004 | 0 | 0 | **0.00385** |  |
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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **T1** | | | | | |  |  |
| **sample name** | Sample\_1 | Sample\_2 | Sample\_3 | Sample\_4 | Sample\_5 | Sample\_6 | **Average** |  |
| 1-Methyladenosine | 0.0031 | 0.0055 | 0.0052 | 0.0063 | 0.0041 | 0.0053 | **0.00491667** |  |
| 1-Methylhistidine | 0.0065 | 0.0059 | 0.0059 | 0.0079 | 0.0045 | 0.0046 | **0.00588333** |  |
| 2-Aminooctanoic acid | 0.0163 | 0.0084 | 0.0133 | 0.0335 | 0.0157 | 0.0196 | **0.0178** |  |
| 2-Furoic acid | 0.1721 | 0.4265 | 0.3265 | 0.069 | 0.2164 | 0.1966 | **0.23451667** |  |
| 2-Isopropylmalic acid | 0.006 | 0.0087 | 0.0095 | 0.0086 | 0.0066 | 0.0087 | **0.00801667** |  |
| 2-Methyl-3-ketovaleric acid | 0.2337 | 0.1949 | 0.2433 | 0.1149 | 0.055 | 0.0613 | **0.15051667** |  |
| 2-Methylglutaric acid | 0.0078 | 0.0149 | 0.0324 | 0.0064 | 0.0058 | 0.0102 | **0.01291667** |  |
| 2-Piperidinone | 0.0067 | 0.0313 | 0.3033 | 0.0235 | 0.0285 | 0.0025 | **0.06596667** |  |
| 2-Pyrrolidinone | 0.0011 | 0.0022 | 0.0068 | 0.0011 | 0.0015 | 0.0007 | **0.00223333** |  |
| 3-Indolepropionic acid | 0.0234 | 0.0523 | 0.0439 | 0.0217 | 0.0099 | 0.0221 | **0.02888333** |  |
| 3-Methoxybenzenepropanoic acid | 0.0145 | 0.028 | 0.0197 | 0.0127 | 0.0086 | 0.0078 | **0.01521667** |  |
| 3-Methylindole | 0.0185 | 0.0298 | 0.0576 | 0.0207 | 0.0249 | 0.0159 | **0.0279** |  |
| 5-Hydroxyindoleacetic acid | 0.0013 | 0.0013 | 0.0014 | 0.0039 | 0.0006 | 0.0009 | **0.00156667** |  |
| 7-Methylguanine | 0.0051 | 0.0079 | 0.0068 | 0.0074 | 0.0065 | 0.0077 | **0.0069** |  |
| Acetylglycine | 0.0019 | 0.0031 | 0.0023 | 0.0191 | 0.0018 | 0.0027 | **0.00515** |  |
| Allantoin | 0.0878 | 0.1367 | 0.0994 | 0.0428 | 0.0441 | 0.0376 | **0.07473333** |  |
| Ascorbic acid | 0.0258 | 0.0352 | 0.0349 | 0.0265 | 0.0205 | 0.0263 | **0.0282** |  |
| Asymmetric dimethylarginine and Symmetric dimethylarginine | 0.0334 | 0.0467 | 0.0416 | 0.0314 | 0.0302 | 0.0255 | **0.0348** |  |
| Azelaic acid | 0.2804 | 0.624 | 0.5927 | 0.1714 | 0.1653 | 0.1911 | **0.33748333** |  |
| Betaine | 0.5918 | 1.0867 | 0.7888 | 1.5055 | 1.3683 | 1.7154 | **1.17608333** |  |
| Butyric acid | 0.0023 | 0.0053 | 0.0021 | 0.003 | 0.0015 | 0.007 | **0.00353333** |  |
| C10H19N3O5 | 0.0111 | 0.0201 | 0.0123 | 0.017 | 0.0102 | 0.0134 | **0.01401667** |  |
| C10H7NO2 | 0.0059 | 0.0109 | 0.0101 | 0.0055 | 0.0132 | 0.0086 | **0.00903333** |  |
| C10H9NO3 | 0.0253 | 0.0473 | 0.0519 | 0.0108 | 0.0413 | 0.0412 | **0.0363** |  |
| C11H19NO9 | 0.0034 | 0.0054 | 0.0006 | 0.0009 | 0.0087 | 0.0006 | **0.00326667** |  |
| C18H39NO2 | 0.0009 | 0.0008 | 0.0017 | 0.0013 | 0.0009 | 0.0019 | **0.00125** |  |
| C24H38O5 | 0.3458 | 0.2538 | 0.2195 | 0.1132 | 0.0977 | 0.0258 | **0.17596667** |  |
| C33H36N4O6 | 0 | 0 | 0.0057 | 0 | 0 | 0.0148 | **0.00341667** |  |
| C5H10O5 | 0.0099 | 0.0176 | 0.0132 | 0.0099 | 0.0104 | 0.0136 | **0.01243333** |  |
| C6H10O6 | 0.0218 | 0.0315 | 0.0293 | 0.0223 | 0.0178 | 0.0217 | **0.02406667** |  |
| C6H8N2O2 | 0.0045 | 0.0097 | 0.0116 | 0.0108 | 0.007 | 0.0069 | **0.00841667** |  |
| C6H8O4 | 0.0013 | 0.0027 | 0.0017 | 0.0055 | 0.0026 | 0.0021 | **0.00265** |  |
| C9H10N2O5 | 0.0005 | 0.0011 | 0.0007 | 0.0007 | 0.0009 | 0.0015 | **0.0009** |  |
| C9H13NO | 0.037 | 0.0709 | 0.311 | 0.0572 | 0.0477 | 0.0981 | **0.10365** |  |
| C9H13NO3 | 0.0345 | 0.1446 | 0.0321 | 0.0091 | 0.0079 | 0.004 | **0.0387** |  |
| C9H6O2 | 0.0249 | 0.0339 | 0.0502 | 0.0137 | 0.0223 | 0.0141 | **0.02651667** |  |
| C9H9NO4 | 0.0023 | 0.0031 | 0.0047 | 0.0025 | 0.0018 | 0.004 | **0.00306667** |  |
| Carvone | 0.0113 | 0.0194 | 0.036 | 0.0171 | 0.0111 | 0.0182 | **0.01885** |  |
| Cholic acid | 5.3378 | 12.4865 | 18.8017 | 1.7845 | 1.3868 | 2.0629 | **6.9767** |  |
| Choline | 0.054 | 0.0851 | 0.0745 | 0.1051 | 0.0724 | 0.0742 | **0.07755** |  |
| Cinnamic acid | 0.1498 | 0.2086 | 0.231 | 0.1412 | 0.1141 | 0.0984 | **0.15718333** |  |
| Citric acid | 0.5754 | 1.4408 | 1.0772 | 0.2188 | 0.7356 | 0.6369 | **0.78078333** |  |
| Citrulline | 0.0233 | 0.0332 | 0.0305 | 0.0183 | 0.0316 | 0.0198 | **0.02611667** |  |
| Creatine | 0.5959 | 0.9677 | 0.8423 | 0.8526 | 0.793 | 0.7149 | **0.7944** |  |
| Creatinine | 0.098 | 0.1743 | 0.1191 | 0.1706 | 0.1249 | 0.121 | **0.13465** |  |
| Cytosine | 0.0016 | 0.1332 | 0.1287 | 0.077 | 0.0627 | 0.0568 | **0.07666667** |  |
| Deoxycytidine | 0 | 0.0098 | 0.0073 | 0.0032 | 0.0045 | 0.0017 | **0.00441667** |  |
| Desaminotyrosine | 0.0759 | 0.139 | 0.0529 | 0.0181 | 0.0289 | 0.013 | **0.05463333** |  |
| Dimethyl sulfone | 0.0088 | 0.0159 | 0.0059 | 0.0015 | 0.0031 | 0.0011 | **0.00605** |  |
| Dimethylmalonic acid | 0.0064 | 0.0148 | 0.0074 | 0.004 | 0.0048 | 0.0047 | **0.00701667** |  |
| Disaccaride - C12H22O11 | 0.0147 | 0.0279 | 0.0247 | 0.0173 | 0.019 | 0.0247 | **0.02138333** |  |
| Fumaric acid | 0.013 | 0.0253 | 0.0261 | 0.0081 | 0.0054 | 0.0058 | **0.01395** |  |
| Galacturonic acid | 0.0302 | 0.0441 | 0.0424 | 0.0315 | 0.0247 | 0.0296 | **0.03375** |  |
| Gluconic acid | 0.0272 | 0.0429 | 0.0448 | 0.0393 | 0.0436 | 0.0284 | **0.0377** |  |
| Glycerophosphocholine | 0.0149 | 0.0172 | 0.0335 | 0.0185 | 0.0216 | 0.0164 | **0.02035** |  |
| Glycocholic acid | 2.7239 | 1.5209 | 1.095 | 0.4762 | 0.4617 | 0.747 | **1.17078333** |  |
| Hippuric acid | 2.638 | 5.76 | 3.311 | 1.2773 | 1.0063 | 0.8816 | **2.47903333** |  |
| Homocitrulline | 0.001 | 0.0018 | 0.0013 | 0.0017 | 0.0013 | 0.001 | **0.00135** |  |
| Hydroxyisobutyric acid | 0.0317 | 0.0571 | 0.0155 | 0.0094 | 0.0126 | 0.0114 | **0.02295** |  |
| Hydroxyphenyllactic acid | 0.0731 | 0.1352 | 0.0758 | 0.0523 | 0.0304 | 0.0292 | **0.066** |  |
| Hypoxantine | 0.051 | 0.0753 | 0.0528 | 0.0505 | 0.0515 | 0.0332 | **0.05238333** |  |
| Indoleacetic acid | 0.0014 | 0.0018 | 0.0018 | 0.0023 | 0.0013 | 0.0023 | **0.00181667** |  |
| Indoleacrylic acid | 0.0069 | 0.0166 | 0.0319 | 0.0022 | 0.0014 | 0.0016 | **0.0101** |  |
| Indolelactic acid | 0.6358 | 1.0479 | 2.0037 | 0.7617 | 0.8868 | 0.5638 | **0.98328333** |  |
| Kynurenine | 0.0364 | 0.0626 | 0.0834 | 0.0596 | 0.0638 | 0.0403 | **0.05768333** |  |
| L-Acetylcarnitine | 0.0287 | 0.0639 | 0.0516 | 0.0263 | 0.0698 | 0.0484 | **0.04811667** |  |
| Lactic acid | 0.0796 | 0.165 | 0.1052 | 0.3575 | 0.1508 | 0.1315 | **0.16493333** |  |
| L-Alanine | 0.4249 | 0.5455 | 0.2777 | 0.4482 | 0.1752 | 0.4081 | **0.37993333** |  |
| L-Arginine | 0.0051 | 0.0079 | 0.007 | 0.0067 | 0.0064 | 0.006 | **0.00651667** |  |
| L-Carnitine | 0.1173 | 0.1584 | 0.2132 | 0.1172 | 0.152 | 0.1184 | **0.14608333** |  |
| L-Glutamic acid | 0.095 | 0.1337 | 0.1138 | 0.1466 | 0.1882 | 0.1693 | **0.1411** |  |
| L-Glutamine | 0.0106 | 0.015 | 0.0206 | 0.0115 | 0.013 | 0.0098 | **0.01341667** |  |
| L-Histidine | 0.0077 | 0.0114 | 0.0168 | 0.0102 | 0.0144 | 0.0079 | **0.0114** |  |
| L-Leucine + L-Isoleucine | 0.0086 | 0.011 | 0.0234 | 0.0105 | 0.0076 | 0.0112 | **0.01205** |  |
| L-Lysine | 0.3383 | 0.4187 | 0.6581 | 0.2558 | 0.2843 | 0.216 | **0.36186667** |  |
| L-Methionine | 0.0032 | 0.0035 | 0.0059 | 0.0022 | 0.0036 | 0.002 | **0.0034** |  |
| L-Phenylalanine | 0.0422 | 0.0631 | 0.0862 | 0.0348 | 0.0538 | 0.0316 | **0.05195** |  |
| L-Proline | 0.3865 | 0.5299 | 0.705 | 0.4479 | 0.3918 | 0.3064 | **0.46125** |  |
| L-Threonine | 0.1067 | 0.1449 | 0.1798 | 0.1416 | 0.2035 | 0.1414 | **0.15298333** |  |
| L-Tryptophan | 0.0009 | 0.0017 | 0.0038 | 0.0016 | 0.002 | 0.0011 | **0.00185** |  |
| L-Tyrosine | 0.1446 | 0.2425 | 0.521 | 0.1741 | 0.2033 | 0.1211 | **0.23443333** |  |
| L-Valine | 0.1304 | 0.1915 | 0.2712 | 0.0716 | 0.1155 | 0.0716 | **0.14196667** |  |
| Malic acid | 0.1264 | 0.1628 | 0.2525 | 0.0925 | 0.0992 | 0.1248 | **0.14303333** |  |
| Mesaconic acid | 0.0413 | 0.0826 | 0.084 | 0.0274 | 0.0174 | 0.0182 | **0.04515** |  |
| Monosaccaride - C6H12O6 | 0.0118 | 0.0265 | 0.0211 | 0.0162 | 0.0146 | 0.0122 | **0.01706667** |  |
| N-Acetyl-L-phenylalanine | 0.1108 | 0.065 | 0.0582 | 0.0415 | 0.0419 | 0.05 | **0.06123333** |  |
| Niacinamide | 0.0124 | 0.0184 | 0.0172 | 0.0291 | 0.0058 | 0.0158 | **0.01645** |  |
| Nutriacholic acid | 0.084 | 0.2002 | 0.1815 | 0.0668 | 0.0919 | 0.0821 | **0.11775** |  |
| Ornithine | 0.0884 | 0.1977 | 0.3894 | 0.037 | 0.0245 | 0.0502 | **0.1312** |  |
| Oxoglutaric acid | 0.1174 | 0.1706 | 0.1119 | 0.0704 | 0.1101 | 0.0708 | **0.10853333** |  |
| Pantothenic acid | 0.0716 | 0.1136 | 0.0765 | 0.0524 | 0.0381 | 0.0259 | **0.06301667** |  |
| Phenylacetaldehyde | 0.0085 | 0.0136 | 0.0258 | 0.0163 | 0.0142 | 0.0153 | **0.01561667** |  |
| Phenylacetylglycine | 0.016 | 0.0236 | 0.031 | 0.0079 | 0.0117 | 0.0083 | **0.01641667** |  |
| Pipecolic acid | 1.0642 | 3.0941 | 1.1692 | 0.6276 | 0.3541 | 0.2563 | **1.09425** |  |
| Pyroglutamic acid | 0.0142 | 0.0216 | 0.0171 | 0.0431 | 0.0448 | 0.0191 | **0.02665** |  |
| Riboflavin | 0.096 | 0.1498 | 0.1316 | 0.0825 | 0.1237 | 0.0768 | **0.11006667** |  |
| Ribothymidine | 0.0016 | 0.0037 | 0.0033 | 0.0029 | 0.0017 | 0.0023 | **0.00258333** |  |
| Sebacic acid | 0.0187 | 0.023 | 0.0261 | 0.0185 | 0.0108 | 0.0225 | **0.01993333** |  |
| Suberic acid | 0.0804 | 0.1994 | 0.1313 | 0.0504 | 0.0518 | 0.0505 | **0.09396667** |  |
| Succinic acid | 0.042 | 0.0819 | 0.1075 | 0.0414 | 0.0283 | 0.0394 | **0.05675** |  |
| Succinic acid semialdehyde | 0.0296 | 0.0523 | 0.0551 | 0.0243 | 0.0218 | 0.0186 | **0.03361667** |  |
| Taurine | 0.0113 | 0.0186 | 0.0125 | 0.008 | 0.0058 | 0.0038 | **0.01** |  |
| Taurocholic acid | 0.0053 | 0.0102 | 0.02 | 0.0141 | 0.0085 | 0.0077 | **0.01096667** |  |
| Taurodeoxycholic acid | 0.4117 | 0.2491 | 0.084 | 0.341 | 0.2918 | 0.773 | **0.35843333** |  |
| Thymidine | 0.4251 | 0.1049 | 0.0548 | 0.3002 | 0.4877 | 1.2644 | **0.43951667** |  |
| Thymine | 0.0359 | 0.0524 | 0.0821 | 0.0534 | 0.0202 | 0.0595 | **0.05058333** |  |
| Traumatic acid | 0.0065 | 0.0115 | 0.0127 | 0.0098 | 0.0067 | 0.0089 | **0.00935** |  |
| Uracil | 0.0104 | 0.0278 | 0.0225 | 0.0118 | 0.0065 | 0.0051 | **0.01401667** |  |
| Uric Acid | 0.0016 | 0.017 | 0.0179 | 0.0077 | 0.0049 | 0.0082 | **0.00955** |  |
| Uridine | 0.1969 | 0.3512 | 0.2724 | 0.185 | 0.1166 | 0.1418 | **0.21065** |  |

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|  | **T2** | | | | | |  |  |
| **sample name** | Sample\_1 | Sample\_2 | Sample\_3 | Sample\_4 | Sample\_5 | Sample\_6 | **Average** |  |
| 1-Methyladenosine | 0.0013 | 0.0029 | 0.0027 | 0.0023 | 0.002 | 0.0015 | **0.00211667** |  |
| 1-Methylhistidine | 0.0084 | 0.0089 | 0.0084 | 0.0055 | 0.0058 | 0.0067 | **0.00728333** |  |
| 2-Aminooctanoic acid | 0.0022 | 0.0017 | 0.0022 | 0.0015 | 0.0012 | 0.0014 | **0.0017** |  |
| 2-Furoic acid | 0.2718 | 0.3417 | 0.404 | 0.2081 | 0.3957 | 0.1568 | **0.29635** |  |
| 2-Isopropylmalic acid | 0.0064 | 0.0111 | 0.0051 | 0.0055 | 0.011 | 0.0025 | **0.00693333** |  |
| 2-Methyl-3-ketovaleric acid | 0.0066 | 0.0055 | 0.0075 | 0.0051 | 0.0086 | 0.0121 | **0.00756667** |  |
| 2-Methylglutaric acid | 0.0961 | 0.1082 | 0.1468 | 0.0718 | 0.1062 | 0.0693 | **0.09973333** |  |
| 2-Piperidinone | 0.0065 | 0.0097 | 0.0163 | 0.0036 | 0.0061 | 0.0052 | **0.0079** |  |
| 2-Pyrrolidinone | 0.0015 | 0.0018 | 0.0015 | 0.0012 | 0.0012 | 0.0008 | **0.00133333** |  |
| 3-Indolepropionic acid | 0 | 0.0008 | 0.0009 | 0.0009 | 0.0005 | 0 | **0.00051667** |  |
| 3-Methoxybenzenepropanoic acid | 0.0263 | 0.04 | 0.0134 | 0.0103 | 0.0145 | 0.0052 | **0.01828333** |  |
| 3-Methylindole | 0.0096 | 0.02 | 0.0194 | 0.0096 | 0.0152 | 0.01 | **0.01396667** |  |
| 5-Hydroxyindoleacetic acid | 0.0129 | 0.0253 | 0.0369 | 0.0143 | 0.0237 | 0.0212 | **0.02238333** |  |
| 7-Methylguanine | 0.0007 | 0.0018 | 0.0011 | 0.0004 | 0.0006 | 0.0017 | **0.00105** |  |
| Acetylglycine | 0.0018 | 0.0034 | 0.0026 | 0.0019 | 0.0021 | 0.0015 | **0.00221667** |  |
| Allantoin | 0.0016 | 0.0021 | 0.0017 | 0.0009 | 0.0014 | 0.0018 | **0.00158333** |  |
| Ascorbic acid | 0.0389 | 0.0501 | 0.0777 | 0.0363 | 0.0593 | 0.0342 | **0.04941667** |  |
| Asymmetric dimethylarginine and Symmetric dimethylarginine | 0.0178 | 0.0258 | 0.0329 | 0.0173 | 0.0244 | 0.0172 | **0.02256667** |  |
| Azelaic acid | 0.0191 | 0.0313 | 0.0308 | 0.0218 | 0.0236 | 0.0194 | **0.02433333** |  |
| Betaine | 0.2282 | 0.3713 | 0.5058 | 0.3006 | 0.4137 | 0.2505 | **0.34501667** |  |
| Butyric acid | 0.4899 | 1.105 | 0.9813 | 0.6265 | 0.7379 | 0.7745 | **0.78585** |  |
| C10H19N3O5 | 0.0052 | 0.0056 | 0.0148 | 0.0034 | 0.0074 | 0.0041 | **0.00675** |  |
| C10H7NO2 | 0.0076 | 0.0145 | 0.0142 | 0.0096 | 0.0106 | 0.0102 | **0.01111667** |  |
| C10H9NO3 | 0.0042 | 0.0068 | 0.0059 | 0.0032 | 0.0056 | 0.0035 | **0.00486667** |  |
| C11H19NO9 | 0.0131 | 0.0259 | 0.0244 | 0.0093 | 0.0289 | 0.014 | **0.01926667** |  |
| C18H39NO2 | 0.0027 | 0.0065 | 0.0097 | 0.0091 | 0.0012 | 0.0003 | **0.00491667** |  |
| C24H38O5 | 0.0006 | 0.0013 | 0.0011 | 0.0012 | 0.0012 | 0.0012 | **0.0011** |  |
| C33H36N4O6 | 0.8287 | 1.0383 | 0.977 | 1.0191 | 2.4196 | 2.0574 | **1.39001667** |  |
| C5H10O5 | 0.0061 | 0.0089 | 0.0098 | 0.005 | 0.0088 | 0.0049 | **0.00725** |  |
| C6H10O6 | 0.0143 | 0.0215 | 0.0264 | 0.0124 | 0.0208 | 0.0144 | **0.0183** |  |
| C6H8N2O2 | 0.0027 | 0.0045 | 0.0042 | 0.0023 | 0.0036 | 0.0028 | **0.00335** |  |
| C6H8O4 | 0.0015 | 0.0022 | 0.0053 | 0.0033 | 0.0019 | 0.001 | **0.00253333** |  |
| C9H10N2O5 | 0.0551 | 0.1145 | 0.0427 | 0.0527 | 0.0356 | 0.0427 | **0.05721667** |  |
| C9H13NO | 0.2405 | 0.3575 | 0.0329 | 0.1754 | 0.4883 | 0.03 | **0.22076667** |  |
| C9H13NO3 | 0.0147 | 0.0266 | 0.0383 | 0.0168 | 0.023 | 0.0168 | **0.0227** |  |
| C9H6O2 | 0.0011 | 0.0027 | 0.003 | 0.0014 | 0.0023 | 0.0019 | **0.00206667** |  |
| C9H9NO4 | 0.0112 | 0.023 | 0.0144 | 0.0143 | 0.0131 | 0.0143 | **0.01505** |  |
| Carvone | 5.7169 | 10.6836 | 11.5709 | 6.5376 | 12.3474 | 7.6673 | **9.08728333** |  |
| Cholic acid | 0.0423 | 0.068 | 0.1035 | 0.0617 | 0.0606 | 0.0556 | **0.06528333** |  |
| Choline | 0.07 | 0.1132 | 0.1709 | 0.0707 | 0.1068 | 0.0661 | **0.09961667** |  |
| Cinnamic acid | 0.8488 | 1.0774 | 1.2383 | 0.6245 | 1.1618 | 0.4782 | **0.90483333** |  |
| Citric acid | 0.0124 | 0.0154 | 0.0154 | 0.0119 | 0.0141 | 0.0149 | **0.01401667** |  |
| Citrulline | 0.6122 | 1.0332 | 1.1281 | 0.8204 | 0.7002 | 0.6535 | **0.8246** |  |
| Creatine | 0.0977 | 0.1696 | 0.1478 | 0.1095 | 0.1342 | 0.1014 | **0.1267** |  |
| Creatinine | 0.0249 | 0.0503 | 0.0585 | 0.0409 | 0.0438 | 0.0346 | **0.04216667** |  |
| Cytosine | 0.0013 | 0.0023 | 0.003 | 0.0029 | 0.0021 | 0.0017 | **0.00221667** |  |
| Deoxycytidine | 0.0082 | 0.0139 | 0.0106 | 0.0068 | 0.0128 | 0.0053 | **0.0096** |  |
| Desaminotyrosine | 0.0005 | 0.0007 | 0.0012 | 0.0004 | 0.0004 | 0.0004 | **0.0006** |  |
| Dimethyl sulfone | 0.0032 | 0.006 | 0.0083 | 0.0032 | 0.0035 | 0.0024 | **0.00443333** |  |
| Dimethylmalonic acid | 0.0083 | 0.0155 | 0.0157 | 0.0084 | 0.0093 | 0.0055 | **0.01045** |  |
| Disaccaride - C12H22O11 | 0.0054 | 0.009 | 0.0119 | 0.0074 | 0.0055 | 0.0037 | **0.00715** |  |
| Fumaric acid | 0.0201 | 0.0303 | 0.0404 | 0.0186 | 0.0309 | 0.0208 | **0.02685** |  |
| Galacturonic acid | 0.0207 | 0.0274 | 0.0954 | 0.0268 | 0.0269 | 0.0151 | **0.03538333** |  |
| Gluconic acid | 0.011 | 0.0179 | 0.029 | 0.016 | 0.0151 | 0.0157 | **0.01745** |  |
| Glycerophosphocholine | 0.2122 | 0.9782 | 1.2145 | 0.5647 | 0.4406 | 0.571 | **0.66353333** |  |
| Glycocholic acid | 3.5572 | 5.0952 | 4.693 | 2.7858 | 5.0223 | 1.8343 | **3.8313** |  |
| Hippuric acid | 0.0009 | 0.0016 | 0.0016 | 0.0008 | 0.0008 | 0.0007 | **0.00106667** |  |
| Homocitrulline | 0.0153 | 0.0283 | 0.0326 | 0.0263 | 0.037 | 0.01 | **0.02491667** |  |
| Hydroxyisobutyric acid | 0.0613 | 0.0808 | 0.1082 | 0.0402 | 0.0955 | 0.0447 | **0.07178333** |  |
| Hydroxyphenyllactic acid | 0.0186 | 0.0428 | 0.0303 | 0.0199 | 0.0388 | 0.017 | **0.0279** |  |
| Hypoxantine | 0.0004 | 0.0012 | 0.0008 | 0.0008 | 0.0007 | 0.0006 | **0.00075** |  |
| Indoleacetic acid | 0.0013 | 0.0059 | 0.0034 | 0.0013 | 0.0021 | 0.0022 | **0.0027** |  |
| Indoleacrylic acid | 0.4806 | 0.9479 | 1.3318 | 0.5313 | 0.8813 | 0.7687 | **0.8236** |  |
| Indolelactic acid | 0.0224 | 0.0505 | 0.0455 | 0.0177 | 0.0502 | 0.021 | **0.03455** |  |
| Kynurenine | 0.0189 | 0.0338 | 0.028 | 0.0172 | 0.031 | 0.0166 | **0.02425** |  |
| L-Acetylcarnitine | 0.082 | 0.1093 | 0.3091 | 0.1836 | 0.0971 | 0.0591 | **0.14003333** |  |
| Lactic acid | 0.4619 | 0.5474 | 0.1871 | 0.1923 | 0.1017 | 0.1467 | **0.27285** |  |
| L-Alanine | 0.0053 | 0.0091 | 0.0098 | 0.007 | 0.0061 | 0.0054 | **0.00711667** |  |
| L-Arginine | 0.065 | 0.0902 | 0.1132 | 0.0667 | 0.0862 | 0.0715 | **0.08213333** |  |
| L-Carnitine | 0.0712 | 0.1075 | 0.2259 | 0.1534 | 0.076 | 0.0679 | **0.11698333** |  |
| L-Glutamic acid | 0.0083 | 0.0175 | 0.0257 | 0.023 | 0.017 | 0.0115 | **0.01716667** |  |
| L-Glutamine | 0.009 | 0.0118 | 0.0143 | 0.0062 | 0.01 | 0.0101 | **0.01023333** |  |
| L-Histidine | 0.0065 | 0.0113 | 0.0148 | 0.0085 | 0.0115 | 0.0129 | **0.01091667** |  |
| L-Leucine + L-Isoleucine | 0.2192 | 0.2941 | 0.4603 | 0.2363 | 0.3034 | 0.2347 | **0.29133333** |  |
| L-Lysine | 0.0023 | 0.0039 | 0.0046 | 0.0024 | 0.0033 | 0.0029 | **0.00323333** |  |
| L-Methionine | 0.0256 | 0.0447 | 0.0597 | 0.0251 | 0.0461 | 0.0351 | **0.03938333** |  |
| L-Phenylalanine | 0.1763 | 0.3095 | 0.4335 | 0.2074 | 0.2949 | 0.2132 | **0.27246667** |  |
| L-Proline | 0.0742 | 0.1198 | 0.1491 | 0.0753 | 0.099 | 0.0877 | **0.10085** |  |
| L-Threonine | 0.0007 | 0.0016 | 0.0027 | 0.0012 | 0.0012 | 0.0013 | **0.00145** |  |
| L-Tryptophan | 0.109 | 0.2231 | 0.3392 | 0.1259 | 0.2103 | 0.1904 | **0.19965** |  |
| L-Tyrosine | 0.0706 | 0.1224 | 0.1822 | 0.0793 | 0.1074 | 0.0805 | **0.10706667** |  |
| L-Valine | 0.0827 | 0.1338 | 0.1726 | 0.0889 | 0.1356 | 0.1215 | **0.12251667** |  |
| Malic acid | 0.0185 | 0.028 | 0.0381 | 0.0231 | 0.0162 | 0.01 | **0.02231667** |  |
| Mesaconic acid | 0.0119 | 0.0195 | 0.0216 | 0.0109 | 0.0168 | 0.0077 | **0.01473333** |  |
| Monosaccaride - C6H12O6 | 0.0693 | 0.0452 | 0.0494 | 0.0199 | 0.0339 | 0.0226 | **0.04005** |  |
| N-Acetyl-L-phenylalanine | 0.0067 | 0.0168 | 0.0057 | 0.0027 | 0.0062 | 0.0045 | **0.0071** |  |
| Niacinamide | 0.0231 | 0.0455 | 0.0758 | 0.0426 | 0.0409 | 0.0292 | **0.04285** |  |
| Nutriacholic acid | 0.0959 | 0.1657 | 0.2016 | 0.1338 | 0.2183 | 0.1591 | **0.1624** |  |
| Ornithine | 0.0666 | 0.0697 | 0.0686 | 0.0608 | 0.0774 | 0.0608 | **0.06731667** |  |
| Oxoglutaric acid | 0.0657 | 0.0781 | 0.0585 | 0.0295 | 0.0435 | 0.0383 | **0.05226667** |  |
| Pantothenic acid | 0.0025 | 0.0048 | 0.011 | 0.0042 | 0.0047 | 0.0043 | **0.00525** |  |
| Phenylacetaldehyde | 0.0092 | 0.0139 | 0.0221 | 0.009 | 0.0145 | 0.0102 | **0.01315** |  |
| Phenylacetylglycine | 0.5494 | 1.1086 | 0.4475 | 0.4371 | 0.7304 | 0.3937 | **0.61111667** |  |
| Pipecolic acid | 0.0075 | 0.0142 | 0.014 | 0.0078 | 0.0093 | 0.0068 | **0.00993333** |  |
| Pyroglutamic acid | 0.1616 | 0.2163 | 0.1719 | 0.1376 | 0.13 | 0.1109 | **0.15471667** |  |
| Riboflavin | 0.0014 | 0.0038 | 0.0026 | 0.0013 | 0.004 | 0.0018 | **0.00248333** |  |
| Ribothymidine | 0.0065 | 0.0111 | 0.0166 | 0.0084 | 0.0081 | 0.0066 | **0.00955** |  |
| Sebacic acid | 0.0672 | 0.13 | 0.1733 | 0.0991 | 0.1355 | 0.0756 | **0.11345** |  |
| Suberic acid | 0.0392 | 0.0658 | 0.0862 | 0.0507 | 0.0666 | 0.0502 | **0.05978333** |  |
| Succinic acid | 0.0213 | 0.041 | 0.029 | 0.0226 | 0.0145 | 0.0106 | **0.02316667** |  |
| Succinic acid semialdehyde | 0.011 | 0.0136 | 0.0104 | 0.005 | 0.0079 | 0.0063 | **0.00903333** |  |
| Taurine | 0.0036 | 0.0099 | 0.0141 | 0.0112 | 0.005 | 0.0047 | **0.00808333** |  |
| Taurocholic acid | 0.0035 | 0.0152 | 0.0161 | 0.0082 | 0.0064 | 0.0085 | **0.00965** |  |
| Taurodeoxycholic acid | 0.0054 | 0.0266 | 0.0208 | 0.0143 | 0.0147 | 0.0237 | **0.01758333** |  |
| Thymidine | 0.0115 | 0.0165 | 0.0223 | 0.0162 | 0.0187 | 0.0167 | **0.01698333** |  |
| Thymine | 0.0021 | 0.0038 | 0.0044 | 0.0032 | 0.0033 | 0.0026 | **0.00323333** |  |
| Traumatic acid | 0.0123 | 0.0225 | 0.0216 | 0.0111 | 0.0198 | 0.01 | **0.01621667** |  |
| Uracil | 0.0027 | 0.0076 | 0.0093 | 0.0077 | 0.0052 | 0.0031 | **0.00593333** |  |
| Uric Acid | 0.0522 | 0.1304 | 0.1494 | 0.1227 | 0.1032 | 0.064 | **0.10365** |  |
| Uridine | 0.0003 | 0.0009 | 0.0012 | 0.0012 | 0.0006 | 0.0004 | **0.00076667** |  |

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| **EO FED CALVES** | **T 0** | | | | | | |  |
| **sample name** | | sample\_7 | Sample\_8 | Sample\_9 | Sample\_10 | Sample\_11 | Sample\_12 | Sample\_13 | **Average** |
| 1-Methyladenosine | | 0.0192 | 0.0081 | 0.0075 | 0.0056 | 0.0098 | 0.006 | 0.0089 | **0.0093** |
| 1-Methylhistidine | | 0.072 | 0.0151 | 0.0084 | 0.0073 | 0.0083 | 0.0036 | 0.0097 | **0.01777143** |
| 2-Aminooctanoic acid | | 0.0242 | 0.0084 | 0.016 | 0.0099 | 0.01 | 0.0049 | 0.0107 | **0.01201429** |
| 2-Furoic acid | | 1.0727 | 0.4525 | 0.301 | 0.2654 | 0.3191 | 0.1187 | 0.3033 | **0.40467143** |
| 2-Isopropylmalic acid | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | **0** |
| 2-Methyl-3-ketovaleric acid | | 0.0386 | 0.0047 | 0.0038 | 0.0028 | 0.0072 | 0.0025 | 0.0041 | **0.0091** |
| 2-Methylglutaric acid | | 0.504 | 0.1798 | 0.1834 | 0.1359 | 0.1883 | 0.1671 | 0.2267 | **0.22645714** |
| 2-Piperidinone | | 0.0093 | 0.0072 | 0.004 | 0.0028 | 0.0038 | 0.0033 | 0.0069 | **0.00532857** |
| 2-Pyrrolidinone | | 0.0012 | 0.0023 | 0.0071 | 0.0043 | 0.0267 | 0.0046 | 0.0037 | **0.00712857** |
| 3-Indolepropionic acid | | 0.0015 | 0 | 0 | 0.0007 | 0.0013 | 0.0008 | 0.0006 | **0.0007** |
| 3-Methoxybenzenepropanoic acid | | 0.0019 | 0.0011 | 0.0016 | 0.0008 | 0.0021 | 0 | 0.0011 | **0.00122857** |
| 3-Methylindole | | 0.0078 | 0.0035 | 0.0041 | 0.0027 | 0.0141 | 0.0031 | 0.0042 | **0.00564286** |
| 5-Hydroxyindoleacetic acid | | 0.0609 | 0.0533 | 0.0416 | 0.03 | 0.0558 | 0.041 | 0.0303 | **0.0447** |
| 7-Methylguanine | | 0.0199 | 0.0074 | 0.0152 | 0.0069 | 0.0039 | 0.0113 | 0.0021 | **0.00952857** |
| Acetylglycine | | 0.0351 | 0.0209 | 0.0173 | 0.012 | 0.02 | 0.0096 | 0.0188 | **0.0191** |
| Allantoin | | 0.0046 | 0.0029 | 0.0028 | 0.0033 | 0.0019 | 0 | 0.002 | **0.0025** |
| Ascorbic acid | | 0.3836 | 0.1139 | 0.0584 | 0.061 | 0.0738 | 0.0256 | 0.0668 | **0.11187143** |
| Asymmetric dimethylarginine and Symmetric dimethylarginine | | 0.0405 | 0.0307 | 0.0304 | 0.0209 | 0.0316 | 0.025 | 0.0282 | **0.02961429** |
| Azelaic acid | | 0.103 | 0.1157 | 0.0745 | 0.0629 | 0.0829 | 0.045 | 0.0618 | **0.07797143** |
| Betaine | | 0.2233 | 0.1505 | 0.1174 | 0.1046 | 0.1547 | 0.1056 | 0.1607 | **0.14525714** |
| Butyric acid | | 3.4975 | 1.9951 | 1.249 | 0.9143 | 1.2614 | 0.679 | 0.8367 | **1.49042857** |
| C10H19N3O5 | | 0.0068 | 0 | 0 | 0 | 0 | 0 | 0.0011 | **0.00112857** |
| C10H7NO2 | | 0.0313 | 0.0184 | 0.0152 | 0.012 | 0.0212 | 0.0147 | 0.0125 | **0.0179** |
| C10H9NO3 | | 0.0029 | 0.0164 | 0.0067 | 0.0029 | 0.0046 | 0.0016 | 0.0031 | **0.00545714** |
| C11H19NO9 | | 0.0085 | 0.0236 | 0.0214 | 0.0047 | 0.0179 | 0.0034 | 0.0122 | **0.0131** |
| C18H39NO2 | | 0.0065 | 0.0113 | 0.0022 | 0.0149 | 0.0204 | 0.0207 | 0.0137 | **0.01281429** |
| C24H38O5 | | 0.0027 | 0.0029 | 0.0032 | 0.0919 | 0.2765 | 0.1384 | 0.1161 | **0.09024286** |
| C33H36N4O6 | | 0.0038 | 0.0248 | 0.0091 | 0.0261 | 0.0055 | 0.0011 | 0.012 | **0.01177143** |
| C5H10O5 | | 0.0329 | 0.0064 | 0.0701 | 0 | 0.0319 | 0.0099 | 0 | **0.0216** |
| C6H10O6 | | 0.0423 | 0.033 | 0.0186 | 0.0125 | 0.0131 | 0.0062 | 0.0133 | **0.01985714** |
| C6H8N2O2 | | 0.0793 | 0.0259 | 0.0254 | 0.0179 | 0.0267 | 0.0218 | 0.0242 | **0.0316** |
| C6H8O4 | | 0.0948 | 0.0107 | 0.004 | 0.0051 | 0.0105 | 0.0048 | 0.0101 | **0.02** |
| C9H10N2O5 | | 0.0053 | 0.0041 | 0.0046 | 0.0036 | 0.0018 | 0.0014 | 0.0026 | **0.00334286** |
| C9H13NO | | 0.0014 | 0.006 | 0.0019 | 0.0013 | 0.0014 | 0 | 0.0008 | **0.00182857** |
| C9H13NO3 | | 0.1149 | 0.0653 | 0.0495 | 0.0334 | 0.0545 | 0.0592 | 0.0817 | **0.0655** |
| C9H6O2 | | 0.0044 | 0.0023 | 0.0024 | 0.0025 | 0.0004 | 0.0012 | 0.0073 | **0.00292857** |
| C9H9NO4 | | 0.0839 | 0.0339 | 0.029 | 0.0185 | 0.0313 | 0.038 | 0.019 | **0.03622857** |
| Carvone | | 0.3787 | 0.0049 | 0.0115 | 0.004 | 0.0273 | 0.0073 | 0.0425 | **0.06802857** |
| Cholic acid | | 0.0349 | 0.019 | 0.0152 | 0.0108 | 0.0193 | 0.0173 | 0.015 | **0.01878571** |
| Choline | | 0.0131 | 0.3165 | 0.0391 | 0.2171 | 0.2661 | 0.0495 | 0.2568 | **0.16545714** |
| Cinnamic acid | | 0.1743 | 0.1407 | 0.1043 | 0.082 | 0.1426 | 0.1093 | 0.0827 | **0.11941429** |
| Citric acid | | 0.2295 | 0.149 | 0.148 | 0.1135 | 0.1485 | 0.1476 | 0.1319 | **0.15257143** |
| Citrulline | | 3.5968 | 1.5563 | 1.0049 | 0.8775 | 1.0693 | 0.4 | 1.0296 | **1.36205714** |
| Creatine | | 0.041 | 0.0193 | 0.0237 | 0.0105 | 0.0252 | 0.0256 | 0.0218 | **0.02387143** |
| Creatinine | | 0.9909 | 0.6937 | 1.2292 | 1.0742 | 1.7241 | 1.0634 | 1.196 | **1.13878571** |
| Cytosine | | 1.0778 | 0.3073 | 0.1646 | 0.1395 | 0.2853 | 0.1156 | 0.1849 | **0.325** |
| Deoxycytidine | | 0.1416 | 0.1647 | 0.1195 | 0.1001 | 0.1162 | 0.0541 | 0.041 | **0.10531429** |
| Desaminotyrosine | | 0.0069 | 0.0055 | 0.0022 | 0.002 | 0.0016 | 0.0005 | 0.0004 | **0.00272857** |
| Dimethyl sulfone | | 0.124 | 0.0364 | 0.0215 | 0.0162 | 0.0315 | 0.0376 | 0.0276 | **0.04211429** |
| Dimethylmalonic acid | | 0.0039 | 0.0012 | 0.0013 | 0.0022 | 0.005 | 0.0004 | 0.0014 | **0.0022** |
| Disaccaride - C12H22O11 | | 0.0168 | 0.0055 | 0.0034 | 0.0036 | 0.0054 | 0.0025 | 0.0054 | **0.00608571** |
| Fumaric acid | | 0.0171 | 0.0239 | 0.0163 | 0.0092 | 0.0142 | 0.0111 | 0.0095 | **0.01447143** |
| Galacturonic acid | | 0.0324 | 0.0078 | 0.0057 | 0.0049 | 0.0082 | 0.0066 | 0.0071 | **0.01038571** |
| Gluconic acid | | 0.0682 | 0.0383 | 0.0358 | 0.0241 | 0.0359 | 0.0277 | 0.0322 | **0.03745714** |
| Glycerophosphocholine | | 0.0845 | 0.0453 | 0.0433 | 0.0324 | 0.0267 | 0.0346 | 0.048 | **0.04497143** |
| Glycocholic acid | | 0.0217 | 0.0163 | 0.0187 | 0.0148 | 0.0139 | 0.0268 | 0.0143 | **0.01807143** |
| Hippuric acid | | 0.6668 | 2.0647 | 1.5693 | 0.8584 | 1.9593 | 1.0077 | 1.2186 | **1.33497143** |
| Homocitrulline | | 0.3042 | 0.0828 | 0.0619 | 0.0226 | 0.0281 | 0.036 | 0.0512 | **0.08382857** |
| Hydroxyisobutyric acid | | 0.0671 | 0.005 | 0.0021 | 0.0029 | 0.0047 | 0.0011 | 0.0043 | **0.01245714** |
| Hydroxyphenyllactic acid | | 0.0898 | 0.0538 | 0.0568 | 0.0505 | 0.0714 | 0.0477 | 0.065 | **0.06214286** |
| Hypoxantine | | 0.7564 | 0.1027 | 0.0522 | 0.0513 | 0.1241 | 0.0885 | 0.0812 | **0.17948571** |
| Indoleacetic acid | | 0.0047 | 0.0024 | 0.002 | 0.0016 | 0.0024 | 0.0014 | 0.0016 | **0.0023** |
| Indoleacrylic acid | | 0.0052 | 0.0012 | 0.0015 | 0.0003 | 0.004 | 0.001 | 0.0004 | **0.00194286** |
| Indolelactic acid | | 2.049 | 1.8004 | 1.3831 | 0.9812 | 1.8839 | 1.3748 | 1.0185 | **1.4987** |
| Kynurenine | | 1.1728 | 0.2248 | 0.1282 | 0.0971 | 0.2879 | 0.1346 | 0.155 | **0.31434286** |
| L-Acetylcarnitine | | 0.0147 | 0.0682 | 0.0276 | 0.0153 | 0.0193 | 0.0049 | 0.0137 | **0.02338571** |
| Lactic acid | | 0.3224 | 0.2321 | 0.2726 | 0.2149 | 0.1014 | 0.069 | 0.1593 | **0.19595714** |
| L-Alanine | | 1.3707 | 0.5167 | 0.4637 | 0.3914 | 0.3734 | 0.2781 | 0.65 | **0.57771429** |
| L-Arginine | | 0.0102 | 0.0059 | 0.0109 | 0.0094 | 0.0143 | 0.0091 | 0.0105 | **0.01004286** |
| L-Carnitine | | 0.1554 | 0.2552 | 0.3126 | 0.1944 | 0.3146 | 0.287 | 0.179 | **0.2426** |
| L-Glutamic acid | | 0.1689 | 0.1954 | 0.2563 | 0.1366 | 0.1163 | 0.0532 | 0.0911 | **0.1454** |
| L-Glutamine | | 0.0201 | 0.0489 | 0.0381 | 0.0281 | 0.0359 | 0.0367 | 0.024 | **0.03311429** |
| L-Histidine | | 0.051 | 0.0144 | 0.0071 | 0.0042 | 0.0099 | 0 | 0.0057 | **0.01318571** |
| L-Leucine + L-Isoleucine | | 0.0473 | 0.0243 | 0.0399 | 0.0225 | 0.0274 | 0.0354 | 0.0496 | **0.0352** |
| L-Lysine | | 0.5673 | 0.4579 | 0.3443 | 0.2906 | 0.3743 | 0.514 | 0.3465 | **0.41355714** |
| L-Methionine | | 0.0041 | 0.0064 | 0.0046 | 0.0034 | 0.0053 | 0.007 | 0.0024 | **0.00474286** |
| L-Phenylalanine | | 0.1506 | 0.1205 | 0.1264 | 0.0844 | 0.1254 | 0.0984 | 0.1274 | **0.11901429** |
| L-Proline | | 0.8984 | 0.5699 | 0.5076 | 0.38 | 0.5459 | 0.4987 | 0.4248 | **0.54647143** |
| L-Threonine | | 0.6101 | 0.4333 | 0.3351 | 0.217 | 0.2972 | 0.2778 | 0.2486 | **0.34558571** |
| L-Tryptophan | | 0.0029 | 0.007 | 0.0067 | 0.0021 | 0.0049 | 0.003 | 0.0049 | **0.0045** |
| L-Tyrosine | | 0.4005 | 0.346 | 0.2572 | 0.1798 | 0.3493 | 0.2601 | 0.2225 | **0.28791429** |
| L-Valine | | 0.3854 | 0.1491 | 0.1203 | 0.0794 | 0.1351 | 0.1641 | 0.0859 | **0.1599** |
| Malic acid | | 0.3318 | 0.1943 | 0.1335 | 0.1196 | 0.1658 | 0.1964 | 0.1449 | **0.18375714** |
| Mesaconic acid | | 0.1172 | 0.0262 | 0.019 | 0.0179 | 0.0276 | 0.0203 | 0.0265 | **0.03638571** |
| Monosaccaride - C6H12O6 | | 0.045 | 0.0205 | 0.0135 | 0.0162 | 0.0234 | 0.0089 | 0.0183 | **0.02082857** |
| N-Acetyl-L-phenylalanine | | 0.313 | 0.0661 | 0.0609 | 0.0405 | 0.066 | 0.0531 | 0.0564 | **0.09371429** |
| Niacinamide | | 0.0396 | 0.0121 | 0.0165 | 0.0031 | 0.0141 | 0.0074 | 0.0057 | **0.01407143** |
| Nutriacholic acid | | 0.2229 | 0.3299 | 0.3611 | 0.037 | 0.119 | 0.0688 | 0.1987 | **0.19105714** |
| Ornithine | | 0.0062 | 0.0095 | 0.0063 | 0.0045 | 0.0104 | 0.0134 | 0.0075 | **0.00825714** |
| Oxoglutaric acid | | 0.1204 | 0.0507 | 0.074 | 0.0387 | 0.0824 | 0.0944 | 0.0739 | **0.07635714** |
| Pantothenic acid | | 0.0542 | 0.0929 | 0.0918 | 0.0671 | 0.0618 | 0.1079 | 0.1369 | **0.08751429** |
| Phenylacetaldehyde | | 0.4 | 0.0888 | 0.074 | 0.0467 | 0.108 | 0.0473 | 0.0734 | **0.11974286** |
| Phenylacetylglycine | | 0.0315 | 0.0127 | 0.0108 | 0.0078 | 0.0119 | 0.0164 | 0.0093 | **0.01434286** |
| Pipecolic acid | | 0.3101 | 0.0137 | 0.0249 | 0.0124 | 0.0539 | 0.0118 | 0.014 | **0.06297143** |
| Pyroglutamic acid | | 0.0444 | 0.0181 | 0.0262 | 0.0128 | 0.0227 | 0.012 | 0.0142 | **0.02148571** |
| Riboflavin | | 0.3522 | 0.1844 | 0.1185 | 0.0871 | 0.1604 | 0.0672 | 0.112 | **0.15454286** |
| Ribothymidine | | 0.0061 | 0.0205 | 0.0079 | 0.0052 | 0.008 | 0.0029 | 0.0057 | **0.00804286** |
| Sebacic acid | | 0.0275 | 0.0192 | 0.0281 | 0.0162 | 0.0359 | 0.0181 | 0.0533 | **0.02832857** |
| Suberic acid | | 0.1775 | 0.053 | 0.0437 | 0.0368 | 0.0583 | 0.0444 | 0.0491 | **0.06611429** |
| Succinic acid | | 0.0696 | 0.036 | 0.028 | 0.0268 | 0.0395 | 0.0298 | 0.0451 | **0.03925714** |
| Succinic acid semialdehyde | | 0.0555 | 0.0375 | 0.0271 | 0.0337 | 0.0375 | 0.0485 | 0.0417 | **0.04021429** |
| Taurine | | 0.0079 | 0.0135 | 0.0126 | 0.01 | 0.0103 | 0.0187 | 0.0195 | **0.01321429** |
| Taurocholic acid | | 0.1563 | 0.029 | 0.0261 | 0.0179 | 0.022 | 0.012 | 0.0178 | **0.04015714** |
| Taurodeoxycholic acid | | 0.2435 | 0.8176 | 0.3653 | 0.2157 | 0.7745 | 0.2088 | 0.3276 | **0.42185714** |
| Thymidine | | 0.4275 | 0.1893 | 0.0933 | 0.0454 | 0.4339 | 0.0706 | 0.0937 | **0.19338571** |
| Thymine | | 0.4852 | 0.0843 | 0.1626 | 0.2256 | 0.0535 | 0.0188 | 0.0228 | **0.1504** |
| Traumatic acid | | 0.0933 | 0.0296 | 0.0291 | 0.0443 | 0.0197 | 0.0062 | 0.0087 | **0.03298571** |
| Uracil | | 0.1724 | 0.0113 | 0.0247 | 0.0219 | 0.0247 | 0.0202 | 0.0307 | **0.0437** |
| Uric Acid | | 0.0068 | 0.0143 | 0.0169 | 0.0111 | 0.0217 | 0.0112 | 0.0221 | **0.01487143** |
| Uridine | | 0.5987 | 0.4186 | 0.2475 | 0.1935 | 0.3512 | 0.1769 | 0.1988 | **0.31217143** |
|  | | 0 | 0.0017 | 0.0021 | 0.0011 | 0.002 | 0.0016 | 0.0029 | **0.00162857** |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **T 1** | | | | | | |  |
| **sample name** | Sample\_7 | Sample\_8 | Sample\_9 | Sample\_10 | Sample\_11 | Sample\_12 | Sample\_13 | **Average** |
| 1-Methyladenosine | 0.0042 | 0.0033 | 0.0028 | 0.0063 | 0.005 | 0.0029 | 0.0032 | **0.00395714** |
| 1-Methylhistidine | 0.0066 | 0.005 | 0.0046 | 0.0066 | 0.0083 | 0.0047 | 0.0054 | **0.00588571** |
| 2-Aminooctanoic acid | 0.0227 | 0.0175 | 0.0301 | 0.0317 | 0.0185 | 0.0151 | 0.0125 | **0.02115714** |
| 2-Furoic acid | 0.1838 | 0.155 | 0.0123 | 0.6119 | 0.2249 | 0.1658 | 0.1998 | **0.22192857** |
| 2-Isopropylmalic acid | 0.0016 | 0.0018 | 0 | 0.0026 | 0 | 0 | 0.0013 | **0.00104286** |
| 2-Methyl-3-ketovaleric acid | 0.0075 | 0.0071 | 0.0024 | 0.0093 | 0.0081 | 0.005 | 0.0073 | **0.00667143** |
| 2-Methylglutaric acid | 0.0739 | 0.1244 | 0.0365 | 0.1659 | 0.0986 | 0.1099 | 0.1349 | **0.1063** |
| 2-Piperidinone | 0.0075 | 0.0102 | 0.0024 | 0.0104 | 0.0064 | 0.0061 | 0.0045 | **0.00678571** |
| 2-Pyrrolidinone | 0.0462 | 0.0507 | 0.103 | 0.2698 | 0.1159 | 0.0012 | 0.0043 | **0.08444286** |
| 3-Indolepropionic acid | 0.001 | 0.0014 | 0.0016 | 0.0026 | 0.0022 | 0.0007 | 0.001 | **0.0015** |
| 3-Methoxybenzenepropanoic acid | 0.0224 | 0.0236 | 0.008 | 0.0092 | 0.0095 | 0.0049 | 0.0055 | **0.01187143** |
| 3-Methylindole | 0.013 | 0.0097 | 0.0036 | 0.0119 | 0.0078 | 0.0104 | 0.0052 | **0.0088** |
| 5-Hydroxyindoleacetic acid | 0.0246 | 0.0262 | 0.0199 | 0.0438 | 0.0264 | 0.0175 | 0.0161 | **0.02492857** |
| 7-Methylguanine | 0.0018 | 0.0016 | 0.0008 | 0.0021 | 0.0019 | 0.001 | 0.0007 | **0.00141429** |
| Acetylglycine | 0.0071 | 0.0055 | 0.0059 | 0.0097 | 0.009 | 0.0046 | 0.0059 | **0.00681429** |
| Allantoin | 0.0017 | 0.002 | 0.0018 | 0.0031 | 0.0025 | 0.0019 | 0.0012 | **0.00202857** |
| Ascorbic acid | 0.0604 | 0.0734 | 0.0194 | 0.0907 | 0.057 | 0.0446 | 0.0473 | **0.05611429** |
| Asymmetric dimethylarginine and Symmetric dimethylarginine | 0.0223 | 0.0273 | 0.0166 | 0.0402 | 0.0251 | 0.0197 | 0.0167 | **0.02398571** |
| Azelaic acid | 0.0365 | 0.0321 | 0.0177 | 0.0545 | 0.0472 | 0.0236 | 0.0295 | **0.03444286** |
| Betaine | 0.2922 | 0.3203 | 0.1009 | 0.2937 | 0.2217 | 0.2316 | 0.168 | **0.23262857** |
| Butyric acid | 1.167 | 0.735 | 1.0028 | 1.9638 | 1.5189 | 0.7352 | 0.5199 | **1.0918** |
| C10H19N3O5 | 0.0013 | 0.0024 | 0 | 0.0017 | 0.0011 | 0.002 | 0.0011 | **0.00137143** |
| C10H7NO2 | 0.0121 | 0.0121 | 0.0122 | 0.0159 | 0.0147 | 0.0106 | 0.007 | **0.01208571** |
| C10H9NO3 | 0.0083 | 0.0066 | 0.0041 | 0.0153 | 0.0135 | 0.0051 | 0.01 | **0.00898571** |
| C11H19NO9 | 0.0394 | 0.0398 | 0.0122 | 0.0536 | 0.0488 | 0.0219 | 0.0396 | **0.03647143** |
| C18H39NO2 | 0.0042 | 0.0004 | 0.0027 | 0.0035 | 0.0011 | 0.0027 | 0.003 | **0.00251429** |
| C24H38O5 | 0.0009 | 0.001 | 0.001 | 0.0019 | 0.0019 | 0.0006 | 0.0006 | **0.00112857** |
| C33H36N4O6 | 0.0794 | 0.2867 | 0.0038 | 2.8602 | 0.1139 | 0.1427 | 0.1135 | **0.51431429** |
| C5H10O5 | 0 | 0.0007 | 0 | 0.0071 | 0.0058 | 0 | 0.0099 | **0.00335714** |
| C6H10O6 | 0.0132 | 0.0108 | 0.0068 | 0.0162 | 0.0302 | 0.0084 | 0.0058 | **0.01305714** |
| C6H8N2O2 | 0.0196 | 0.022 | 0.0133 | 0.0343 | 0.0222 | 0.0168 | 0.0139 | **0.0203** |
| C6H8O4 | 0.0082 | 0.0077 | 0.0034 | 0.0094 | 0.0083 | 0.0071 | 0.0045 | **0.00694286** |
| C9H10N2O5 | 0.0018 | 0.0023 | 0.0022 | 0.0033 | 0.0031 | 0.002 | 0.002 | **0.00238571** |
| C9H13NO | 0.0011 | 0.0007 | 0 | 0.0009 | 0.001 | 0.0006 | 0 | **0.00061429** |
| C9H13NO3 | 0.0509 | 0.0628 | 0.0358 | 0.0808 | 0.0442 | 0.0284 | 0.0236 | **0.04664286** |
| C9H6O2 | 0.0197 | 0.0479 | 0.0016 | 0.0243 | 0.0052 | 0.0475 | 0.0033 | **0.02135714** |
| C9H9NO4 | 0.0239 | 0.0245 | 0.0105 | 0.0415 | 0.0273 | 0.0185 | 0.0243 | **0.02435714** |
| Carvone | 0.0026 | 0.0025 | 0.0014 | 0.0031 | 0.0027 | 0.0013 | 0.0029 | **0.00235714** |
| Cholic acid | 0.0126 | 0.0172 | 0.0111 | 0.0166 | 0.0155 | 0.0089 | 0.0075 | **0.01277143** |
| Choline | 6.4183 | 3.3956 | 0.3716 | 12.2208 | 1.0712 | 2.0337 | 2.2769 | **3.96972857** |
| Cinnamic acid | 0.0795 | 0.0656 | 0.0516 | 0.1672 | 0.1387 | 0.057 | 0.0511 | **0.08724286** |
| Citric acid | 0.1302 | 0.1638 | 0.103 | 0.2151 | 0.1406 | 0.1161 | 0.1016 | **0.13862857** |
| Citrulline | 0.5941 | 0.5024 | 0.0438 | 1.9916 | 0.7288 | 0.5425 | 0.6468 | **0.72142857** |
| Creatine | 0.0243 | 0.0218 | 0.0111 | 0.0409 | 0.0342 | 0.0194 | 0.0159 | **0.02394286** |
| Creatinine | 0.7812 | 0.7154 | 0.4606 | 1.2595 | 1.1008 | 0.6035 | 0.6526 | **0.79622857** |
| Cytosine | 0.126 | 0.1165 | 0.1018 | 0.1803 | 0.1726 | 0.0937 | 0.133 | **0.13198571** |
| Deoxycytidine | 0.0817 | 0.1079 | 0.0444 | 0.0847 | 0.0773 | 0.0465 | 0.056 | **0.07121429** |
| Desaminotyrosine | 0.0051 | 0.0058 | 0.0013 | 0.0091 | 0.0043 | 0.0026 | 0.0054 | **0.0048** |
| Dimethyl sulfone | 0.0295 | 0.0224 | 0.0159 | 0.0754 | 0.0235 | 0.0128 | 0.0404 | **0.03141429** |
| Dimethylmalonic acid | 0.003 | 0.0026 | 0.0017 | 0.0007 | 0.001 | 0.0046 | 0.0017 | **0.00218571** |
| Disaccaride - C12H22O11 | 0.0076 | 0.0048 | 0.0022 | 0.0069 | 0.0037 | 0.0047 | 0.0029 | **0.00468571** |
| Fumaric acid | 0.015 | 0.0194 | 0.0124 | 0.0372 | 0.0258 | 0.0104 | 0.0217 | **0.02027143** |
| Galacturonic acid | 0.0057 | 0.0071 | 0.0027 | 0.0108 | 0.0068 | 0.008 | 0.0082 | **0.00704286** |
| Gluconic acid | 0.0271 | 0.0313 | 0.0179 | 0.0492 | 0.0307 | 0.0224 | 0.0196 | **0.02831429** |
| Glycerophosphocholine | 0.0375 | 0.0342 | 0.0267 | 0.0496 | 0.0442 | 0.032 | 0.026 | **0.03574286** |
| Glycocholic acid | 0.0233 | 0.0196 | 0.009 | 0.0427 | 0.034 | 0.0158 | 0.0086 | **0.02185714** |
| Hippuric acid | 0.5539 | 1.8579 | 0.8435 | 3.3818 | 4.4849 | 0.4071 | 1.5704 | **1.87135714** |
| Homocitrulline | 1.29 | 2.9766 | 0.2919 | 1.3667 | 0.8808 | 2.2302 | 1.012 | **1.43545714** |
| Hydroxyisobutyric acid | 0.0015 | 0.001 | 0.0015 | 0.0018 | 0.0034 | 0.0012 | 0.0014 | **0.00168571** |
| Hydroxyphenyllactic acid | 0.04 | 0.053 | 0.0121 | 0.0469 | 0.028 | 0.0435 | 0.0278 | **0.0359** |
| Hypoxantine | 0.0318 | 0.0371 | 0.0156 | 0.0746 | 0.037 | 0.0346 | 0.0479 | **0.0398** |
| Indoleacetic acid | 0.0013 | 0.0016 | 0.0022 | 0.0025 | 0.0019 | 0.001 | 0.0015 | **0.00171429** |
| Indoleacrylic acid | 0.0081 | 0.0064 | 0.0005 | 0.0059 | 0.0064 | 0.0014 | 0.0019 | **0.00437143** |
| Indolelactic acid | 0.8822 | 0.9346 | 0.7062 | 1.5061 | 0.9502 | 0.6311 | 0.5814 | **0.88454286** |
| Kynurenine | 0.0383 | 0.0435 | 0.0345 | 0.0916 | 0.0513 | 0.0312 | 0.0371 | **0.04678571** |
| L-Acetylcarnitine | 0.0495 | 0.0395 | 0.0279 | 0.09 | 0.0677 | 0.0253 | 0.0518 | **0.05024286** |
| Lactic acid | 0.1105 | 0.1401 | 0.138 | 0.2156 | 0.201 | 0.1274 | 0.1176 | **0.15002857** |
| L-Alanine | 0.1697 | 0.4305 | 0.1211 | 0.3612 | 0.4829 | 0.3695 | 0.1736 | **0.30121429** |
| L-Arginine | 0.0066 | 0.0059 | 0.0036 | 0.01 | 0.0091 | 0.0046 | 0.0055 | **0.00647143** |
| L-Carnitine | 0.136 | 0.1079 | 0.0524 | 0.2249 | 0.1576 | 0.1107 | 0.0753 | **0.12354286** |
| L-Glutamic acid | 0.154 | 0.1465 | 0.171 | 0.2421 | 0.1744 | 0.1246 | 0.0808 | **0.1562** |
| L-Glutamine | 0.0127 | 0.0128 | 0.0062 | 0.0167 | 0.014 | 0.0089 | 0.0063 | **0.01108571** |
| L-Histidine | 0.0122 | 0.0106 | 0.0037 | 0.0191 | 0.0152 | 0.0065 | 0.0076 | **0.0107** |
| L-Leucine + L-Isoleucine | 0.0103 | 0.0137 | 0.0075 | 0.0146 | 0.0128 | 0.0069 | 0.0082 | **0.01057143** |
| L-Lysine | 0.3156 | 0.3648 | 0.1471 | 0.5753 | 0.3689 | 0.2414 | 0.2604 | **0.32478571** |
| L-Methionine | 0.0028 | 0.0039 | 0.0015 | 0.007 | 0.006 | 0.0023 | 0.0041 | **0.00394286** |
| L-Phenylalanine | 0.0498 | 0.0606 | 0.0234 | 0.1126 | 0.0573 | 0.0316 | 0.0466 | **0.05455714** |
| L-Proline | 0.413 | 0.4645 | 0.4035 | 0.6897 | 0.4794 | 0.3519 | 0.3319 | **0.4477** |
| L-Threonine | 0.1338 | 0.0993 | 0.0968 | 0.2704 | 0.1998 | 0.0851 | 0.1281 | **0.14475714** |
| L-Tryptophan | 0.0014 | 0.0017 | 0.0008 | 0.0027 | 0.0017 | 0.0011 | 0.0018 | **0.0016** |
| L-Tyrosine | 0.2233 | 0.2304 | 0.169 | 0.3836 | 0.2251 | 0.1506 | 0.142 | **0.21771429** |
| L-Valine | 0.1284 | 0.1324 | 0.0524 | 0.2293 | 0.1471 | 0.0989 | 0.1251 | **0.13051429** |
| Malic acid | 0.116 | 0.1291 | 0.0646 | 0.1948 | 0.1407 | 0.0971 | 0.0932 | **0.11935714** |
| Mesaconic acid | 0.0197 | 0.0232 | 0.0083 | 0.0367 | 0.022 | 0.0266 | 0.0255 | **0.02314286** |
| Monosaccaride - C6H12O6 | 0.0105 | 0.0104 | 0.0038 | 0.0288 | 0.0186 | 0.0111 | 0.0131 | **0.01375714** |
| N-Acetyl-L-phenylalanine | 0.0398 | 0.0447 | 0.0283 | 0.0727 | 0.0477 | 0.0356 | 0.0323 | **0.04301429** |
| Niacinamide | 0.0149 | 0.0215 | 0.0069 | 0.0271 | 0.0283 | 0.0122 | 0.0072 | **0.01687143** |
| Nutriacholic acid | 0.1156 | 0.0788 | 0.0143 | 0.1371 | 0.0389 | 0.095 | 0.0581 | **0.07682857** |
| Ornithine | 0.1152 | 0.0695 | 0.012 | 0.2553 | 0.0409 | 0.0393 | 0.0483 | **0.08292857** |
| Oxoglutaric acid | 0.0968 | 0.0886 | 0.0305 | 0.1445 | 0.1283 | 0.0832 | 0.0555 | **0.08962857** |
| Pantothenic acid | 0.0514 | 0.0626 | 0.0178 | 0.0507 | 0.046 | 0.0589 | 0.0283 | **0.0451** |
| Phenylacetaldehyde | 0.0132 | 0.0097 | 0.0197 | 0.0196 | 0.0183 | 0.0077 | 0.012 | **0.01431429** |
| Phenylacetylglycine | 0.0145 | 0.0164 | 0.0052 | 0.0238 | 0.0149 | 0.0117 | 0.0115 | **0.014** |
| Pipecolic acid | 0.9478 | 1.264 | 0.1829 | 0.7585 | 0.3326 | 0.6519 | 0.2203 | **0.62257143** |
| Pyroglutamic acid | 0.016 | 0.01 | 0.0098 | 0.0184 | 0.0346 | 0.0677 | 0.0076 | **0.02344286** |
| Riboflavin | 0.1048 | 0.0989 | 0.0502 | 0.1519 | 0.1164 | 0.0853 | 0.0789 | **0.09805714** |
| Ribothymidine | 0.0018 | 0.0023 | 0.0015 | 0.0046 | 0.0055 | 0.0011 | 0.0023 | **0.00272857** |
| Sebacic acid | 0.0137 | 0.0152 | 0.0126 | 0.0196 | 0.0144 | 0.0153 | 0.0116 | **0.01462857** |
| Suberic acid | 0.0819 | 0.0896 | 0.0322 | 0.0906 | 0.0628 | 0.0518 | 0.0635 | **0.06748571** |
| Succinic acid | 0.0359 | 0.0452 | 0.021 | 0.055 | 0.041 | 0.0357 | 0.0318 | **0.03794286** |
| Succinic acid semialdehyde | 0.0204 | 0.0184 | 0.0121 | 0.0197 | 0.0156 | 0.029 | 0.0169 | **0.01887143** |
| Taurine | 0.009 | 0.0106 | 0.0027 | 0.0088 | 0.0078 | 0.0088 | 0.0051 | **0.00754286** |
| Taurocholic acid | 0.0106 | 0.0091 | 0.0086 | 0.0196 | 0.0191 | 0.0046 | 0.0105 | **0.01172857** |
| Taurodeoxycholic acid | 0.2523 | 0.8061 | 0.4798 | 1.3966 | 4.1205 | 0.0739 | 0.8097 | **1.13412857** |
| Thymidine | 0.1887 | 1.3715 | 0.5278 | 1.2503 | 5.7161 | 0.1287 | 1.4773 | **1.52291429** |
| Thymine | 0.026 | 0.0862 | 0.0152 | 0.041 | 0.0734 | 0.0322 | 0.0264 | **0.04291429** |
| Traumatic acid | 0.0077 | 0.0103 | 0.0042 | 0.0097 | 0.012 | 0.006 | 0.0053 | **0.00788571** |
| Uracil | 0.0128 | 0.0116 | 0.0086 | 0.0103 | 0.0067 | 0.0101 | 0.0066 | **0.00952857** |
| Uric Acid | 0.0064 | 0.0088 | 0.0064 | 0.0058 | 0.0064 | 0.0057 | 0.0041 | **0.00622857** |
| Uridine | 0.1698 | 0.2413 | 0.0815 | 0.1885 | 0.2004 | 0.1585 | 0.1043 | **0.16347143** |
|  | 0.0008 | 0.0011 | 0.0007 | 0.0008 | 0.0008 | 0.0007 | 0.0005 | **0.00077143** |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **T 2** | | | | | | |  |
| **sample name** | Sample\_7 | Sample\_8 | Sample\_9 | Sample\_10 | Sample\_11 | Sample\_12 | Sample\_13 | **Average** |
| 1-Methyladenosine | 0.0011 | 0.0014 | 0.003 | 0.0011 | 0.0015 | 0.0018 | 0.0015 | **0.00162857** |
| 1-Methylhistidine | 0.0046 | 0.0035 | 0.0067 | 0.0033 | 0.006 | 0.0078 | 0.0042 | **0.00515714** |
| 2-Aminooctanoic acid | 0.0027 | 0.0016 | 0.0031 | 0.0008 | 0.0015 | 0.0016 | 0.0024 | **0.00195714** |
| 2-Furoic acid | 0.0902 | 0.1864 | 0.2813 | 0.1511 | 0.3046 | 0.1671 | 0.2015 | **0.19745714** |
| 2-Isopropylmalic acid | 0.0018 | 0.0012 | 0.004 | 0 | 0.0065 | 0.0027 | 0.0044 | **0.00294286** |
| 2-Methyl-3-ketovaleric acid | 0.0036 | 0.0044 | 0.006 | 0.0043 | 0.0094 | 0.0047 | 0.0058 | **0.00545714** |
| 2-Methylglutaric acid | 0.0878 | 0.0727 | 0.1034 | 0.0355 | 0.0775 | 0.0531 | 0.0535 | **0.06907143** |
| 2-Piperidinone | 0.0094 | 0.0056 | 0.01 | 0.0032 | 0.0066 | 0.0062 | 0.0041 | **0.00644286** |
| 2-Pyrrolidinone | 0.0003 | 0.0006 | 0 | 0.0005 | 0.0009 | 0.0008 | 0.0007 | **0.00054286** |
| 3-Indolepropionic acid | 0 | 0 | 0.0005 | 0 | 0 | 0 | 0 | **7.1429E-05** |
| 3-Methoxybenzenepropanoic acid | 0.013 | 0.0106 | 0.0212 | 0.0205 | 0.0113 | 0.018 | 0.0093 | **0.01484286** |
| 3-Methylindole | 0.0108 | 0.0105 | 0.0222 | 0.0083 | 0.0145 | 0.0119 | 0.0129 | **0.01301429** |
| 5-Hydroxyindoleacetic acid | 0.0144 | 0.0198 | 0.0234 | 0.0095 | 0.0147 | 0.0198 | 0.0189 | **0.01721429** |
| 7-Methylguanine | 0.0005 | 0.0005 | 0.0047 | 0.0007 | 0.0004 | 0 | 0.0007 | **0.00107143** |
| Acetylglycine | 0.0011 | 0.0015 | 0.0029 | 0.001 | 0.0018 | 0.0019 | 0.0016 | **0.00168571** |
| Allantoin | 0.0012 | 0.0011 | 0.0018 | 0.0007 | 0.002 | 0.0014 | 0.0013 | **0.00135714** |
| Ascorbic acid | 0.0214 | 0.0345 | 0.0558 | 0.0298 | 0.0439 | 0.0358 | 0.0427 | **0.0377** |
| Asymmetric dimethylarginine and Symmetric dimethylarginine | 0.0145 | 0.0148 | 0.0277 | 0.0144 | 0.0189 | 0.0168 | 0.0166 | **0.01767143** |
| Azelaic acid | 0.0129 | 0.0176 | 0.0312 | 0.0132 | 0.0254 | 0.0215 | 0.0185 | **0.02004286** |
| Betaine | 0.2668 | 0.231 | 0.5487 | 0.2606 | 0.3841 | 0.3153 | 0.3866 | **0.34187143** |
| Butyric acid | 0.4188 | 0.5078 | 1.1288 | 0.4407 | 0.6436 | 0.8312 | 0.4289 | **0.62854286** |
| C10H19N3O5 | 0.0049 | 0.0076 | 0.0108 | 0.0027 | 0.0092 | 0.0041 | 0.0049 | **0.00631429** |
| C10H7NO2 | 0.0041 | 0.0066 | 0.0152 | 0.007 | 0.0098 | 0.0109 | 0.0069 | **0.00864286** |
| C10H9NO3 | 0.0022 | 0.0044 | 0.0059 | 0.0027 | 0.0058 | 0.0043 | 0.005 | **0.00432857** |
| C11H19NO9 | 0.0089 | 0.019 | 0.0194 | 0.0097 | 0.0307 | 0.018 | 0.0227 | **0.01834286** |
| C18H39NO2 | 0.0004 | 0.0008 | 0.0014 | 0.0007 | 0.0014 | 0.0026 | 0.0003 | **0.00108571** |
| C24H38O5 | 0.0007 | 0.0008 | 0.0016 | 0.0007 | 0.0011 | 0.0011 | 0.0005 | **0.00092857** |
| C33H36N4O6 | 0.8251 | 1.3792 | 0.5918 | 1.95 | 0.9219 | 1.3626 | 0.5783 | **1.08698571** |
| C5H10O5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | **0** |
| C6H10O6 | 0.0035 | 0.0046 | 0.0093 | 0.0039 | 0.0062 | 0.005 | 0.0055 | **0.00542857** |
| C6H8N2O2 | 0.0122 | 0.0124 | 0.0228 | 0.0117 | 0.0163 | 0.0141 | 0.0134 | **0.0147** |
| C6H8O4 | 0.0018 | 0.0019 | 0.0037 | 0.0018 | 0.0028 | 0.0031 | 0.0022 | **0.00247143** |
| C9H10N2O5 | 0.0009 | 0.0007 | 0.0016 | 0.0005 | 0.0011 | 0.0015 | 0.0006 | **0.00098571** |
| C9H13NO | 0 | 0 | 0 | 0 | 0 | 0 | 0 | **0** |
| C9H13NO3 | 0.0878 | 0.0263 | 0.053 | 0.0318 | 0.0486 | 0.0391 | 0.0225 | **0.04415714** |
| C9H6O2 | 0.0447 | 0.036 | 0.1934 | 0.1102 | 0.1567 | 0.0782 | 0.1065 | **0.10367143** |
| C9H9NO4 | 0.012 | 0.0155 | 0.0335 | 0.014 | 0.0166 | 0.02 | 0.02 | **0.0188** |
| Carvone | 0.0016 | 0.0012 | 0.0019 | 0.0007 | 0.002 | 0.0016 | 0.0014 | **0.00148571** |
| Cholic acid | 0.0114 | 0.0081 | 0.0167 | 0.0095 | 0.0127 | 0.012 | 0.0075 | **0.01112857** |
| Choline | 4.241 | 8.964 | 11.4182 | 9.6539 | 8.0608 | 10.0722 | 7.514 | **8.56058571** |
| Cinnamic acid | 0.0331 | 0.0393 | 0.0863 | 0.0364 | 0.0407 | 0.065 | 0.043 | **0.04911429** |
| Citric acid | 0.0849 | 0.079 | 0.1381 | 0.0659 | 0.0824 | 0.0921 | 0.0919 | **0.09061429** |
| Citrulline | 0.2703 | 0.5643 | 0.8749 | 0.469 | 0.922 | 0.5143 | 0.6066 | **0.60305714** |
| Creatine | 0.0054 | 0.0111 | 0.0169 | 0.0084 | 0.0101 | 0.0104 | 0.0097 | **0.01028571** |
| Creatinine | 0.3453 | 0.5096 | 1.0399 | 0.3701 | 0.6266 | 0.6491 | 0.5182 | **0.57982857** |
| Cytosine | 0.0542 | 0.0758 | 0.1408 | 0.0623 | 0.0929 | 0.0927 | 0.0838 | **0.08607143** |
| Deoxycytidine | 0.0239 | 0.028 | 0.0558 | 0.0324 | 0.0358 | 0.0258 | 0.036 | **0.03395714** |
| Desaminotyrosine | 0.0023 | 0.0019 | 0.0035 | 0.0029 | 0.0029 | 0.0018 | 0.0034 | **0.00267143** |
| Dimethyl sulfone | 0.0054 | 0.0049 | 0.0086 | 0.0054 | 0.0107 | 0.0072 | 0.0071 | **0.00704286** |
| Dimethylmalonic acid | 0.0005 | 0.0002 | 0.0005 | 0.0002 | 0.0006 | 0.0003 | 0.0003 | **0.00037143** |
| Disaccaride - C12H22O11 | 0.0019 | 0.0029 | 0.0052 | 0.0021 | 0.0038 | 0.0033 | 0.0033 | **0.00321429** |
| Fumaric acid | 0.0075 | 0.0048 | 0.0114 | 0.0046 | 0.0099 | 0.0117 | 0.0052 | **0.00787143** |
| Galacturonic acid | 0.0033 | 0.0028 | 0.0057 | 0.0023 | 0.0033 | 0.0047 | 0.0036 | **0.00367143** |
| Gluconic acid | 0.0175 | 0.0183 | 0.0332 | 0.0166 | 0.0239 | 0.0207 | 0.0211 | **0.02161429** |
| Glycerophosphocholine | 0.0142 | 0.0143 | 0.0259 | 0.0138 | 0.0184 | 0.0133 | 0.0182 | **0.01687143** |
| Glycocholic acid | 0.0098 | 0.0111 | 0.021 | 0.0105 | 0.0109 | 0.0104 | 0.0134 | **0.01244286** |
| Hippuric acid | 0.2743 | 0.5364 | 2.0935 | 0.2841 | 0.5198 | 0.7776 | 1.0634 | **0.79272857** |
| Homocitrulline | 1.5624 | 2.2383 | 7.2434 | 3.2022 | 3.5189 | 2.7645 | 3.1746 | **3.38632857** |
| Hydroxyisobutyric acid | 0.0006 | 0.0004 | 0.0013 | 0.0003 | 0.0009 | 0.0007 | 0.0007 | **0.0007** |
| Hydroxyphenyllactic acid | 0.042 | 0.0441 | 0.0797 | 0.0423 | 0.083 | 0.0449 | 0.0522 | **0.05545714** |
| Hypoxantine | 0.012 | 0.0159 | 0.0295 | 0.017 | 0.0267 | 0.0202 | 0.022 | **0.02047143** |
| Indoleacetic acid | 0.0003 | 0.0004 | 0.0009 | 0 | 0.0006 | 0 | 0.0006 | **0.0004** |
| Indoleacrylic acid | 0.0012 | 0.0034 | 0.0043 | 0.0014 | 0.0062 | 0.0028 | 0.0045 | **0.0034** |
| Indolelactic acid | 0.526 | 0.7108 | 0.8765 | 0.3533 | 0.5425 | 0.6945 | 0.6523 | **0.62227143** |
| Kynurenine | 0.017 | 0.0225 | 0.0253 | 0.0143 | 0.0332 | 0.0309 | 0.0257 | **0.02412857** |
| L-Acetylcarnitine | 0.0116 | 0.0232 | 0.0294 | 0.0134 | 0.0307 | 0.0228 | 0.0287 | **0.02282857** |
| Lactic acid | 0.0483 | 0.0456 | 0.093 | 0.0317 | 0.0551 | 0.0874 | 0.0417 | **0.05754286** |
| L-Alanine | 0.2152 | 0.1541 | 0.173 | 0.0673 | 0.1359 | 0.1929 | 0.086 | **0.14634286** |
| L-Arginine | 0.0028 | 0.0041 | 0.0086 | 0.0031 | 0.0053 | 0.0054 | 0.0042 | **0.00478571** |
| L-Carnitine | 0.0355 | 0.0535 | 0.103 | 0.0463 | 0.0667 | 0.0812 | 0.0545 | **0.06295714** |
| L-Glutamic acid | 0.0522 | 0.0553 | 0.1134 | 0.0411 | 0.0559 | 0.0826 | 0.0533 | **0.06482857** |
| L-Glutamine | 0.0076 | 0.0089 | 0.022 | 0.0076 | 0.0103 | 0.0086 | 0.0093 | **0.01061429** |
| L-Histidine | 0.0057 | 0.0088 | 0.0165 | 0.0058 | 0.0115 | 0.0139 | 0.0086 | **0.01011429** |
| L-Leucine + L-Isoleucine | 0.0086 | 0.009 | 0.0157 | 0.0066 | 0.0104 | 0.0092 | 0.0095 | **0.00985714** |
| L-Lysine | 0.217 | 0.2224 | 0.4208 | 0.1915 | 0.2736 | 0.2556 | 0.2715 | **0.26462857** |
| L-Methionine | 0.0024 | 0.0027 | 0.0051 | 0.0022 | 0.0032 | 0.0029 | 0.0028 | **0.00304286** |
| L-Phenylalanine | 0.0245 | 0.0311 | 0.0635 | 0.025 | 0.0249 | 0.038 | 0.0343 | **0.03447143** |
| L-Proline | 0.2156 | 0.202 | 0.4136 | 0.1677 | 0.1945 | 0.2484 | 0.2255 | **0.23818571** |
| L-Threonine | 0.0625 | 0.0667 | 0.1439 | 0.0484 | 0.0767 | 0.0806 | 0.0763 | **0.0793** |
| L-Tryptophan | 0.0012 | 0.0012 | 0.0018 | 0.0006 | 0.0009 | 0.0015 | 0.0019 | **0.0013** |
| L-Tyrosine | 0.1384 | 0.1896 | 0.2124 | 0.0834 | 0.1322 | 0.1762 | 0.1814 | **0.15908571** |
| L-Valine | 0.0591 | 0.0794 | 0.1666 | 0.071 | 0.0831 | 0.0977 | 0.102 | **0.09412857** |
| Malic acid | 0.0844 | 0.0945 | 0.1699 | 0.0718 | 0.1024 | 0.1088 | 0.1105 | **0.10604286** |
| Mesaconic acid | 0.0096 | 0.0087 | 0.018 | 0.0062 | 0.011 | 0.0143 | 0.01 | **0.01111429** |
| Monosaccaride - C6H12O6 | 0.0054 | 0.0084 | 0.0132 | 0.0074 | 0.0136 | 0.0083 | 0.0093 | **0.00937143** |
| N-Acetyl-L-phenylalanine | 0.02 | 0.0196 | 0.0438 | 0.018 | 0.0322 | 0.0288 | 0.0231 | **0.0265** |
| Niacinamide | 0.0076 | 0.0051 | 0.0134 | 0.0039 | 0.0074 | 0.0073 | 0.0081 | **0.00754286** |
| Nutriacholic acid | 0.03 | 0.0238 | 0.0465 | 0.0195 | 0.0238 | 0.028 |  | **0.0286** |
| Ornithine | 0.0748 | 0.1591 | 0.2068 | 0.1662 | 0.1123 | 0.1858 | 0.1296 | **0.1478** |
| Oxoglutaric acid | 0.0305 | 0.047 | 0.0799 | 0.0389 | 0.0627 | 0.0542 | 0.054 | **0.05245714** |
| Pantothenic acid | 0.0477 | 0.0283 | 0.0617 | 0.0178 | 0.032 | 0.0271 | 0.0253 | **0.03427143** |
| Phenylacetaldehyde | 0.0032 | 0.0033 | 0.0056 | 0.0029 | 0.0035 | 0.0039 | 0.004 | **0.00377143** |
| Phenylacetylglycine | 0.007 | 0.0104 | 0.0193 | 0.0089 | 0.0113 | 0.0117 | 0.0131 | **0.01167143** |
| Pipecolic acid | 0.1554 | 0.29 | 0.5836 | 0.143 | 0.5396 | 0.3208 | 0.3747 | **0.34387143** |
| Pyroglutamic acid | 0.006 | 0.0055 | 0.0142 | 0.0055 | 0.0083 | 0.007 | 0.007 | **0.00764286** |
| Riboflavin | 0.081 | 0.1101 | 0.214 | 0.0822 | 0.1402 | 0.1555 | 0.1113 | **0.12775714** |
| Ribothymidine | 0.001 | 0.0016 | 0.0028 | 0.0027 | 0.0018 | 0.0012 | 0.0015 | **0.0018** |
| Sebacic acid | 0.0073 | 0.0072 | 0.0073 | 0.0049 | 0.0067 | 0.0126 | 0.0071 | **0.00758571** |
| Suberic acid | 0.0618 | 0.0791 | 0.1729 | 0.0852 | 0.1283 | 0.093 | 0.1227 | **0.10614286** |
| Succinic acid | 0.0473 | 0.0429 | 0.0954 | 0.0459 | 0.0719 | 0.0582 | 0.0639 | **0.06078571** |
| Succinic acid semialdehyde | 0.0122 | 0.0104 | 0.0214 | 0.0092 | 0.0159 | 0.0212 | 0.0105 | **0.0144** |
| Taurine | 0.0085 | 0.0052 | 0.0103 | 0.0032 | 0.0056 | 0.005 | 0.0044 | **0.00602857** |
| Taurocholic acid | 0.003 | 0.0024 | 0.0079 | 0.0026 | 0.0047 | 0.0045 | 0.0022 | **0.0039** |
| Taurodeoxycholic acid | 0.0059 | 0.0092 | 0.0399 | 0.004 | 0.0073 | 0.0097 | 0.0151 | **0.01301429** |
| Thymidine | 0.0101 | 0.0162 | 0.0795 | 0.0062 | 0.0156 | 0.0147 | 0.0228 | **0.02358571** |
| Thymine | 0.0108 | 0.0124 | 0.0365 | 0.0159 | 0.0167 | 0.0166 | 0.0181 | **0.01814286** |
| Traumatic acid | 0.0017 | 0.0021 | 0.0061 | 0.0024 | 0.0023 | 0.0031 | 0.0021 | **0.00282857** |
| Uracil | 0.008 | 0.0113 | 0.023 | 0.0121 | 0.019 | 0.0122 | 0.0165 | **0.01458571** |
| Uric Acid | 0.0027 | 0.0026 | 0.0049 | 0.0027 | 0.0023 | 0.0071 | 0.0037 | **0.00371429** |
| Uridine | 0.042 | 0.0496 | 0.1184 | 0.0639 | 0.0882 | 0.1053 | 0.0625 | **0.0757** |
|  | 0.0003 | 0.0003 | 0.0005 | 0.0003 | 0.0003 | 0.001 | 0.0005 | **0.00045714** |