Developmental signatures of microbiota-derived metabolites in the mouse brain
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Supplementary Information

Supplementary Figure 1: Principal components analysis (PCA) model constructed on the forebrain metabolic profiles of all study animals. A) Scores plot (PC1 v PC2) and B) loadings plot from the PCA model ($R^2 = 95\%$) using mean centered and pareto scaled data. AMP, adenosine monophosphate; GABA, $\gamma$-aminobutyric acid; GPC, glycerophosphocholine.
**Supplementary Table S1:** Forebrain metabolites significantly different between prepubertal (P21) and postnatal (P3). 121 metabolites were significantly higher in the forebrain of P21 mice compared to P3 mice and 78 metabolites significantly lower. Criteria for significance was greater than two-fold change (P21 relative to P3) and FDR-adjusted *P* < 0.05.

| Metabolite                                      | Fold change (P21 vs. P3) | log2(FC)  | *p* adj  | -Log10(p) |
|-------------------------------------------------|--------------------------|-----------|----------|-----------|
| N-acetylaspartate                               | 4.6362                   | 2.2129    | 1.51E-16 | 15.822    |
| pyroglutamine                                   | 17.699                   | 4.1456    | 2.22E-16 | 15.653    |
| 1,2-dioleoyl-GPC 181/181                       | 5.3136                   | 2.4097    | 3.02E-16 | 15.52     |
| sphingomyelin d181/181, d182/180                | 6.9231                   | 2.7914    | 4.50E-16 | 15.347    |
| 1-stearoyl-2-arachidonoyl-GPC 180/204           | 3.6097                   | 1.8519    | 6.67E-16 | 15.176    |
| cystathionine                                   | 0.24157                  | -2.0495   | 1.57E-15 | 14.803    |
| 1-1-enyl-stearoyl-2-arachidonoyl-GPE P-180/204  | 4.0986                   | 2.0351    | 1.57E-15 | 14.803    |
| xanthine                                        | 4.956                    | 2.3092    | 1.89E-15 | 14.724    |
| putrescine                                      | 0.048905                 | -4.3539   | 2.41E-15 | 14.618    |
| pro-hydroxy-pro                                 | 0.028596                 | -5.1281   | 3.10E-15 | 14.508    |
| carnosine                                       | 7.4746                   | 2.902     | 3.10E-15 | 14.508    |
| sphingosine                                     | 4.2331                   | 2.0817    | 5.05E-15 | 14.297    |
| 1-1-enyl-palmitoyl-2-palmitoyl-GPC 160/160      | 9.6679                   | 3.2732    | 6.53E-15 | 14.185    |
| N-acetyltaurine                                 | 0.10845                  | -3.205    | 9.82E-15 | 14.008    |
| adenine                                         | 4.2115                   | 2.0743    | 9.82E-15 | 14.008    |
| stearoyl sphingomyelin d181/180                 | 8.3916                   | 3.0689    | 1.17E-14 | 13.932    |
| trans-4-hydroxyproline                          | 0.19385                  | -2.367    | 2.17E-14 | 13.665    |
| orotidine                                       | 0.24803                  | -2.0114   | 2.69E-14 | 13.571    |
| homocarnosine                                   | 47585000                 | 25.504    | 2.94E-14 | 13.532    |
| 1,2-dioleoyl-GPE 181/181                       | 3.794                    | 1.9237    | 3.36E-14 | 13.473    |
| 1-1-enyl-palmitoyl-2-oleoyl-GPC 160/161         | 43.796                   | 5.4527    | 3.80E-14 | 13.42     |
| phosphoethanolamine                             | 0.47563                  | -1.0721   | 6.13E-14 | 13.213    |
| desmosterol                                     | 0.13929                  | -2.8438   | 6.75E-14 | 13.17     |
| N-acetylglutamate                               | 5.345                    | 2.4182    | 6.75E-14 | 13.17     |
| 1-1-enyl-palmitoyl-2-arachidonoyl-GPE P-160/204 | 2.5172                   | 1.3318    | 7.36E-14 | 13.133    |
| 7-methylguanine                                 | 0.06562                  | -3.9297   | 1.10E-13 | 12.96     |
| 3-hydroxy-3-methylglutarate                    | 0.32287                  | -1.631    | 1.55E-13 | 12.811    |
| 2′-deoxyctydine                                 | 0.24939                  | -2.0035   | 2.11E-13 | 12.677    |
| N6-carboxyethylthreonyladenosine                | 0.26899                  | -1.8944   | 3.99E-13 | 12.399    |
| 1-1-enyl-stearoyl-2-oleoyl-GPE P-180/181        | 14.717                   | 3.8794    | 4.07E-13 | 12.391    |
| 1-1-enyl-palmitoyl-2-linoleoyl-GPE P-160/182    | 3.0504                   | 1.609     | 4.07E-13 | 12.391    |
| 1,2-dioleoyl-GPC 181/181                       | 2.0284                   | 1.0203    | 4.65E-13 | 12.333    |
| sphingomyelin d181/200, d161/220                | 8.949                    | 3.1617    | 5.12E-13 | 12.291    |
| N-acetylariginine                               | 3.9532                   | 1.983     | 5.12E-13 | 12.291    |
| citrate                                         | 3.9204                   | 1.971     | 5.20E-13 | 12.284    |
| maltotriose                                     | 0.12626                  | -2.9856   | 6.27E-13 | 12.202    |
| N-acetylglutamine                               | 2.5691                   | 1.3612    | 6.65E-13 | 12.177    |
| homoarginine                                    | 0.23484                  | -2.0902   | 8.69E-13 | 12.061    |
| glycosyl-N-stearoyl-sphingosine                 | 6.7299                   | 2.7506    | 8.94E-13 | 12.049    |
| dimethylarginine SDMA ADMA                      | 0.38178                  | -1.3892   | 1.01E-12 | 11.997    |
| sphingomyelin d181/221, d182/220, d161/241      | 4.3887                   | 2.1338    | 1.51E-12 | 11.822    |
| trigonelline                                    | 9.8812                   | 3.3047    | 1.53E-12 | 11.816    |
| 4-imidazolacacetate                             | 0.03481                  | -4.8443   | 1.76E-12 | 11.756    |
| sphingomyelin d181/241, d182/240                | 3.4102                   | 1.7699    | 1.76E-12 | 11.756    |
| maltotetraose                                   | 0.10261                  | -3.2848   | 1.77E-12 | 11.752    |
| Compound                                      | Value 1 | Value 2 | Value 3  | Value 4 | Value 5 |
|-----------------------------------------------|---------|---------|----------|---------|---------|
| N-acetyl methionine                           | 4.384   | 2.1325  | 1.77E-12 | 11.752  |
| anserine                                      | 3.3     | 1.7225  | 1.77E-12 | 11.752  |
| pseudouridine                                 | 0.29254 | -1.7733 | 2.53E-12 | 11.597  |
| 1-palmitoleoyl-GPC 161                        | 0.2421  | -2.0463 | 2.59E-12 | 11.587  |
| γ-glutamyl-c-lysine                           | 0.045241| -4.4662 | 2.94E-12 | 11.531  |
| gulonic acid                                  | 0.075206| -3.733  | 2.95E-12 | 11.53   |
| acetylcholine                                 | 8.4502  | 3.079   | 2.95E-12 | 11.53   |
| 3-sulfo-nervonoyl-galactosylceramide d181/241 | 2128800 | 21.022  | 3.18E-12 | 11.498  |
| 1-stearoyl-GPC 180                            | 2.3743  | 1.2475  | 3.45E-12 | 11.462  |
| sphingomyelin d181/170, d171/180, d191/160    | 11.889  | 3.5715  | 3.94E-12 | 11.404  |
| guanidoacetate                                | 0.13129 | -2.9292 | 6.50E-12 | 11.187  |
| oxalate ethanedioate                          | 0.3813  | -1.391  | 8.01E-12 | 11.096  |
| allantoin                                     | 0.27469 | -1.8641 | 1.27E-11 | 10.897  |
| N-acetylmethane                                | 2.0588  | 1.0418  | 1.27E-11 | 10.897  |
| N-palmitoyl-sphingosine d181/160              | 0.47795 | -1.0651 | 1.29E-11 | 10.899  |
| C-glycosyltryptophan                          | 2.002   | 1.0015  | 1.32E-11 | 10.878  |
| sphingomyelin d181/201, d182/200              | 3.6483  | 1.8672  | 1.37E-11 | 10.863  |
| pyridoxal                                     | 2.1787  | 1.1235  | 1.49E-11 | 10.827  |
| 1-palmitoyl-2-palmitoleoyl-GPC 160/161        | 0.4379  | -1.1913 | 1.54E-11 | 10.811  |
| γ-glutamylglutamate                           | 5.0684  | 2.3415  | 5.55E-11 | 10.809  |
| cholesterol                                   | 3.62    | 1.6651  | 1.86E-11 | 10.69   |
| ornithine                                     | 0.23768 | -2.0729 | 1.76E-11 | 10.749  |
| succinate                                     | 0.27119 | -1.8826 | 1.78E-11 | 10.749  |
| inosine 5'-monophosphate                      | 0.19888 | -2.33   | 2.07E-11 | 10.683  |
| UDP-glucuronate                               | 0.29023 | -1.7847 | 2.45E-11 | 10.611  |
| 2'-deoxyinosine                               | 0.31248 | -1.6782 | 2.57E-11 | 10.59   |
| 1-palmitoyl-2-stearoyl-GPC 160/180            | 2.4824  | 1.3117  | 2.57E-11 | 10.59   |
| threonine                                     | 0.4181  | -1.2581 | 2.59E-11 | 10.56   |
| uridine 5'-monophosphate                      | 0.11992 | -3.0599 | 3.35E-11 | 10.475  |
| 1-palmitoleoyl-2-oleoyl-GPC 161/181           | 0.39027 | -1.3575 | 3.77E-11 | 10.424  |
| palmitoylcarnitine                            | 4.1212  | 2.0431  | 3.82E-11 | 10.418  |
| 2-methylcitrate/homocitrate                  | 2.519   | 1.3328  | 3.82E-11 | 10.418  |
| cytidine 5'-monophosphate                     | 0.4278  | -1.225  | 3.91E-11 | 10.407  |
| N2,N2-dimethylguanosine                       | 0.27814 | -1.8461 | 4.49E-11 | 10.348  |
| cytidine 2',3'-cyclic monophosphate           | 0.34193 | -1.5482 | 4.49E-11 | 10.348  |
| ergothioneine                                 | 0.22421 | -2.1571 | 5.42E-11 | 10.266  |
| 1-1-ethyl-palmitoyl-2-arachidonoyl-GPC P-160/204 | 13.217 | 3.7243  | 5.57E-11 | 10.254  |
| cysteine                                      | 4.3425  | 2.1185  | 5.91E-11 | 10.228  |
| oleoylcarnitine                               | 5.2684  | 2.3964  | 6.29E-11 | 10.201  |
| Pipelicolic acid                              | 0.35955 | -1.4758 | 7.38E-11 | 10.132  |
| guanosine                                     | 3.3152  | 1.7291  | 7.87E-11 | 10.104  |
| γ-glutamylglutamine                           | 2.5648  | 1.3589  | 8.04E-11 | 10.095  |
| pyruvate                                      | 2.9854  | 1.5779  | 9.35E-11 | 10.029  |
| aconitate (cis or trans)                      | 3.5558  | 1.8302  | 1.12E-10 | 9.9494  |
| pyridoxamine phosphate                        | 6.203   | 2.633   | 1.12E-10 | 9.9494  |
| 5-methyl-2'-deoxyctidine                      | 0.30204 | -1.7272 | 1.33E-10 | 9.8754  |
| ribose 1-phosphate                            | 6.9337  | 2.7936  | 2.03E-10 | 9.6927  |
| stearoylcarnitine                             | 3.6565  | 1.8704  | 2.11E-10 | 9.6757  |
| N-palmitoyl-sphinganine d180/160              | 0.26183 | -1.9333 | 2.19E-10 | 9.6598  |
| 2'-deoxyctidine 5'-monophosphate              | 0.34037 | -1.5548 | 2.28E-10 | 9.6414  |
| 1-1-etyl-palmitoyl-2-oleoyl-GPE P-160/181     | 7.2675  | 2.8615  | 2.29E-10 | 9.6398  |
| adenosine 5'-monophosphate                    | 0.42299 | -1.2413 | 2.40E-10 | 9.6196  |
| lactate                                       | 2.1228  | 1.086   | 3.00E-10 | 9.5231  |
| sphingomyelin d182/230, d181/231, d171/241    | 300280  | 18.196  | 3.11E-10 | 9.5072  |
| Substance                                                                 | Value 1  | Value 2  | Value 3  | Value 4  |
|--------------------------------------------------------------------------|---------|---------|---------|---------|
| 1-palmitoyl-2-linoleoyl-GPE 160/182                                      | 0.38938 | -1.3607 | 3.14E-10| 9.5034  |
| citrulline                                                               | 0.39763 | -1.3305 | 3.37E-10| 9.472   |
| β-hydroxyisovalerate                                                     | 0.35645 | -1.4955 | 3.95E-10| 9.4037  |
| saccharopine                                                             | 6508800 | 22.634  | 4.90E-10| 9.3099  |
| glycerol 3-phosphate                                                     | 0.34275 | -1.5448 | 4.90E-10| 9.3099  |
| N-acetyltyrosine                                                         | 0.41322 | -1.275  | 6.15E-10| 9.2111  |
| pyridoxamine                                                             | 4.5081  | 2.1725  | 8.22E-10| 9.0849  |
| guanosine 5'-monophosphate                                               | 0.44088 | -1.1815 | 1.44E-09| 8.8417  |
| cysteineylglycine                                                        | 2.6547  | 1.4085  | 1.45E-09| 8.8399  |
| 3-methylcytidine                                                        | 0.38138 | -1.3907 | 1.50E-09| 8.8234  |
| behenoylsphingomyelin d181/220                                          | 2.2784  | 1.188   | 1.82E-09| 8.7409  |
| uridine 5'-diphosphate                                                   | 0.12475 | -3.0029 | 2.80E-09| 8.5532  |
| adenosine                                                                | 6.8208  | 2.7699  | 2.99E-09| 8.5238  |
| malonylcarnitine                                                        | 3.3321  | 1.7364  | 3.21E-09| 8.4929  |
| N-acetylmethionine sulfoxide                                             | 3.6893  | 1.8834  | 3.37E-09| 8.4729  |
| butyrylcarnitine                                                        | 0.31905 | -1.6481 | 4.07E-09| 8.3905  |
| linoleoylcarnitine                                                       | 4.3051  | 2.106   | 4.28E-09| 8.3684  |
| flavin adenine dinucleotide                                              | 2.0447  | 1.0319  | 4.28E-09| 8.3684  |
| 5-oxoproline                                                            | 2.04    | 1.0286  | 6.19E-09| 8.2086  |
| spermidine                                                              | 0.30457 | -1.7152 | 7.25E-09| 8.1399  |
| N-formylmethionine                                                       | 2.1681  | 1.1165  | 8.68E-09| 8.0617  |
| fructose                                                                | 0.25063 | -1.9964 | 9.62E-09| 8.0167  |
| N-delta-acetylornithine                                                  | 6.1407  | 2.6184  | 1.01E-08| 7.9966  |
| 1-stearoyl-2-oleoyl-GPC 180/181                                          | 2.9262  | 1.549   | 1.08E-08| 7.9657  |
| myristoylcarnitine                                                       | 2.5901  | 1.373   | 1.14E-08| 7.9414  |
| stachydrine                                                             | 2.3057  | 1.2052  | 1.32E-08| 7.879   |
| prostaglandin E2                                                         | 2.85    | 1.5109  | 1.36E-08| 7.865   |
| dimethylglycine                                                          | 0.33703 | -1.5691 | 1.61E-08| 7.7938  |
| glutaryl carnitine C5                                                    | 6.7046  | 2.7451  | 1.77E-08| 7.7511  |
| dehydroascorbate                                                        | 2.4321  | 1.2822  | 1.83E-08| 7.737   |
| thiamin diphosphate                                                      | 2.9459  | 1.5587  | 1.84E-08| 7.7354  |
| 6-phosphogluconate                                                       | 0.28069 | -1.8329 | 2.09E-08| 7.6798  |
| cysteine sulfenic acid                                                   | 15.559  | 3.9597  | 2.32E-08| 7.635   |
| laurycarnitine                                                           | 4.5633  | 2.1901  | 2.45E-08| 7.6116  |
| 2-aminoheptanoate                                                        | 5.0048  | 2.3233  | 2.45E-08| 7.6109  |
| 3-hydroxybutyrate                                                        | 0.28464 | -1.8128 | 2.76E-08| 7.5595  |
| galactonate                                                              | 0.29535 | -1.7595 | 3.04E-08| 7.5165  |
| heme                                                                    | 2.6974  | 1.4136  | 3.87E-08| 7.4126  |
| palmitoylcholine                                                         | 4.7901  | 2.2601  | 6.58E-08| 7.182   |
| 1-palmitoleoyl-3-oleoyl-glycerol 161/181                                  | 0.041627| -4.5864 | 9.57E-08| 7.0191  |
| proline                                                                 | 0.48182 | -1.0534 | 1.04E-07| 6.9841  |
| glucose                                                                  | 0.2469  | -2.018  | 1.19E-07| 6.9253  |
| L-isobar fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate | 0.25113 | -1.9935 | 1.27E-07| 6.8952  |
| N6-carboxymethyllysine                                                   | 3.5522  | 1.8287  | 1.44E-07| 6.8431  |
| adenosine 2'-monophosphate                                               | 0.37507 | -1.4148 | 1.53E-07| 6.8144  |
| γ-glutamyvaline                                                         | 0.4289  | -1.2213 | 1.66E-07| 6.78    |
| 1,2-dilinoleoyl-GPC 182/182                                              | 0.48469 | -1.0449 | 1.82E-07| 6.739   |
| cysteine-glutathione disulfide                                           | 6.6664  | 2.7369  | 2.08E-07| 6.6817  |
| sphingosine 1-phosphate                                                  | 84510   | 16.367  | 2.28E-07| 6.6424  |
| inositol 1-phosphate                                                     | 2.4492  | 1.2923  | 2.96E-07| 6.5288  |
| coenzyme A                                                               | 2.8197  | 1.4956  | 4.77E-07| 6.3217  |
| methylmalonate                                                           | 2.0726  | 1.0514  | 6.85E-07| 6.1644  |
| argininosuccinate                                                        | 2.3416  | 1.2275  | 7.94E-07| 6.1004  |
| Compound                                | Value 1 | Value 2 | Value 3 | Value 4 |
|-----------------------------------------|---------|---------|---------|---------|
| adenosine 5'-diphosphoribose ADP-ribose| 296.84  | 8.2135  | 9.41E-07| 6.0264  |
| cytosine                                | 0.40273 | -1.3121 | 1.07E-06| 5.9715  |
| prostaglandin F2α                       | 2.526   | 1.3369  | 1.33E-06| 5.8747  |
| 1-arachidonoyl-GPI 204                  | 4.5093  | 2.1729  | 1.42E-06| 5.8478  |
| 2-amino adipate                         | 2.2999  | 1.2016  | 1.89E-06| 5.7225  |
| pyridoxal phosphate                     | 2.563   | 1.3578  | 2.30E-06| 5.6375  |
| 2-methylbutyrylcarnitine C5             | 765060  | 19.545  | 2.31E-06| 5.6366  |
| 4-acetamidobutanate                     | 0.4209  | -1.2485 | 2.34E-06| 5.63    |
| 3-hydroxyisobutyrate                    | 0.4529  | -1.1427 | 1.07E-05| 4.9726  |
| 1-1-etyl-oleoyl-GPE P-181              | 2.2525  | 1.1715  | 1.09E-05| 4.9627  |
| N4-acetylcystidine                      | 0.25927 | -1.9475 | 1.47E-05| 4.8327  |
| α-tocopherol                            | 2.9592  | 1.5652  | 1.52E-05| 4.8172  |
| S-lactoylglutathione                    | 7.2943  | 2.8668  | 1.64E-05| 4.7841  |
| 1-oleoyl-GPG 181                        | 17.495  | 4.1289  | 2.06E-05| 4.686   |
| 3-hydroxybutyrylcarnitine 2             | 2.2086  | 1.1431  | 2.53E-05| 4.5961  |
| γ-glutamylhistidine                     | 0.21373 | -2.2261 | 2.94E-05| 4.5314  |
| N-stearoyltaurine                       | 2.3196  | 1.2139  | 4.66E-05| 4.3312  |
| erucate 22:1n9                          | 5.1422  | 2.3624  | 5.11E-05| 4.2915  |
| 1-palmitoyl-GPS 160                     | 0.2838  | -1.817  | 5.49E-05| 4.2603  |
| solanidine                              | 3.9245  | 1.9725  | 7.79E-05| 4.1085  |
| allo-threonine                          | 2.8341  | 1.5029  | 8.31E-05| 4.0806  |
| 1-1-etyl-stearoyl-GPE P-180             | 2.4186  | 1.2741  | 8.36E-05| 4.0777  |
| indolelactate                           | 0.40907 | -1.2896 | 0.00010553| 3.9766 |
| dihydroxyacetone phosphate              | 0.49472 | -1.0153 | 0.00011992| 3.9211 |
| stearate 180                            | 2.5486  | 1.3497  | 0.00013296| 3.8763 |
| guanosine 3'-monophosphate              | 9.9393  | 3.3131  | 0.00013297| 3.8763 |
| oleoyl ethanolamide                     | 5.5757  | 2.4792  | 0.00013672| 3.8642 |
| imidazole propionate                    | 5.7128  | 2.5142  | 0.00017238| 3.7635 |
| 10-nonadecenoate 19:1n9                 | 787210  | 19.586  | 0.00019433| 3.7115 |
| 2-hydroxy-3-methylvalerate              | 3.4332  | 1.7795  | 0.00022024| 3.6571 |
| adenylosuccinate                        | 0.4792  | -1.0613 | 0.00039836| 3.3997 |
| adenosine 5'-diphosphate                | 5.684   | 2.5069  | 0.00043821| 3.3583 |
| eicosenoate 201                         | 3.6288  | 1.8595  | 0.00098573| 3.0062 |
| linolenate α or γ 18:3n3 or 6           | 0.39434 | -1.3425 | 0.0010827| 2.9655 |
| arachidonate 20:4n6                     | 3.4764  | 1.7976  | 0.0011001| 2.9585 |
| adrenate 22:4n6                         | 3.2377  | 1.695   | 0.0012023| 2.92    |
| oleate/vaccenate 181                   | 2.8644  | 1.5183  | 0.0012045| 2.9192 |
| 2'-deoxyadenosine                       | 4.6742  | 2.2247  | 0.0017159| 2.7655 |
| 3-indoxyl sulfate                       | 5.7551  | 2.5248  | 0.0019744| 2.7046 |
| galactose 1-phosphate                   | 0.41487 | -1.2693 | 0.0020376| 2.6909 |
| fructose-6-phosphate                    | 0.42295 | -1.2415 | 0.0026612| 2.5749 |
| 1-palmitoyl-GPG 160                     | 2.135   | 1.0942  | 0.0026651| 2.5743 |
| docosahexaenoate 22:6n3                 | 2.9339  | 1.5528  | 0.0049165| 2.3083 |
| 2-oleoylglycerol 181                    | 3.7374  | 1.902   | 0.0049592| 2.3046 |
| phenol sulfate                          | 6.8315  | 2.7722  | 0.018664| 1.729   |
| docosadienoate 22:2n6                   | 2.3406  | 1.2269  | 0.026193| 1.5818 |
| gluconate                               | 0.48884 | -1.0326 | 0.031631| 1.4999 |
Supplementary Table S2: Forebrain metabolites significantly different between young adult (P60) and prepubertal/juvenile mice (P21). 14 metabolites were significantly higher in the forebrain of P60 mice compared to P21 mice and 29 metabolites significantly lower. Significant metabolites had a greater than two-fold change between the groups (P60 relative to P21) and an FDR-adjusted \(P < 0.05\).

| Metabolite                                | Fold change (P60 vs. P21) | log2(FC) | \(p\)-adj | -LOG10(p) |
|-------------------------------------------|---------------------------|----------|-----------|-----------|
| N-methylnicotinic acid (trigonelline)     | 0.19463                   | -2.3612  | 3.67E-10  | 9.435     |
| stachydrine                               | 0.45015                   | -1.1515  | 4.19E-10  | 9.3774    |
| 4-guanidinobutanoate                      | 0.4767                    | -1.0689  | 4.19E-10  | 9.3774    |
| adenosine                                 | 2.3352                    | 1.2235   | 8.42E-10  | 9.0749    |
| 2'-deoxyctydine                           | 0.36112                   | -1.4694  | 1.30E-08  | 7.8863    |
| 2'-deoxyadenosine                         | 3.5413                    | 1.8243   | 7.61E-08  | 7.1189    |
| sphingomyelin d182/230, d181/231, d171/241| 2.7127                    | 1.4398   | 1.39E-07  | 6.8575    |
| palmitoylcholine                          | 2.2075                    | 1.1424   | 1.53E-07  | 6.8148    |
| allantoin                                 | 0.46968                   | -1.0902  | 2.82E-07  | 6.5501    |
| hypotaurine                               | 0.49554                   | -1.0129  | 2.82E-07  | 6.5501    |
| 7-methylguanine                           | 0.073047                  | -3.775   | 3.34E-07  | 6.4768    |
| ergothioneine                             | 2.2677                    | 1.1812   | 8.73E-07  | 6.0592    |
| dimethylglycine                           | 0.23344                   | -2.0989  | 1.24E-06  | 5.9073    |
| pro-hydroxy-pro                           | 0.42465                   | -1.2356  | 1.24E-06  | 5.9073    |
| 2-aminohexanoate                          | 0.31808                   | 1.6525   | 1.24E-06  | 5.9067    |
| adenosine 2'-monophosphate                | 0.30743                   | -1.7017  | 2.81E-06  | 5.5508    |
| putrescine                                | 0.23335                   | -2.0994  | 3.47E-06  | 5.4601    |
| 5-methyl-2'-deoxyctydine                  | 0.29698                   | -1.7516  | 4.12E-06  | 5.3846    |
| inosine 5'-monophosphate                  | 0.38271                   | -1.3857  | 8.45E-06  | 5.0729    |
| adenosine 5'-diphosphoribose              | 2.2571                    | 1.1745   | 8.46E-06  | 5.0726    |
| uridine 5'-monophosphate                  | 0.42684                   | -1.2282  | 2.97E-05  | 4.5274    |
| 3-methylcytidine                          | 0.3973                    | -1.3317  | 3.07E-05  | 4.5333    |
| cysteinylglycine                          | 2.2831                    | 1.1911   | 3.80E-05  | 4.4198    |
| glutathione                               | 2.1769                    | 1.1223   | 9.05E-05  | 4.0433    |
| 2'-deoxyinosine                           | 0.44955                   | -1.1534  | 9.14E-05  | 4.0389    |
| 4-hydroxy-nonenal-glutathione             | 0.48304                   | -1.0498  | 0.00016992| 3.7698    |
| adenylosuccinate                          | 0.25492                   | -1.9719  | 0.00026016| 3.5848    |
| N4-acetylcysteine                         | 0.21734                   | -2.202   | 0.000335  | 3.475     |
| 3-ureidopropionate                        | 0.49395                   | -1.0176  | 0.00081704| 3.0878    |
| imidazole propionate                      | 0.24348                   | -2.0382  | 0.00085564| 3.0677    |
| palmitoyl ethanolamide                    | 2.5653                    | 1.3591   | 0.00084244| 3.0643    |
| S-lactoylglutathione                      | 2.2332                    | 1.1591   | 0.00099882| 3.0005    |
| cytosine                                  | 0.22993                   | -2.1208  | 0.0010009 | 2.9996    |
| guanosine 3'-monophosphate                | 0.20606                   | -2.2789  | 0.0011251 | 2.9488    |
| urate                                     | 3.3978                    | 1.7646   | 0.001443  | 2.8407    |
| gamma-glutamylglycine                     | 2.0527                    | 1.0375   | 0.0016778 | 2.7753    |
| 2-hydroxy-3-methylvalerate                | 0.40993                   | -1.2865  | 0.0019479 | 2.7104    |
| uridine 5'-diphosphate                    | 0.3935                    | -1.3456  | 0.0020251 | 2.6936    |
| phenol sulfate                            | 3.3664                    | 1.7512   | 0.0038704 | 2.4122    |
| 1-oleoyl-GPG 181                          | 2.1815                    | 1.1253   | 0.0046844 | 2.3327    |
| indolelactate                             | 0.30026                   | -1.7357  | 0.011497  | 1.9394    |
| 1-methylnicotinamide                      | 0.42243                   | -1.2432  | 0.018371  | 1.7359    |
| N-palmitoyltaurine                        | 0.41276                   | -1.2766  | 0.02309   | 1.6366    |