**S1 Table**. **Metabolites studied in this report including their class, ion type, m/z and MT data**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **(M-H)-** | **Annotation** | **KEGG ID** | **HMDB** | **Count/120** | **Avg pm/mg of brain tissue** | ***m/z*** | **MT** | **S/N** | **Detection Limit (pm/mg)** |
| A\_0044 | *N*-Acetylglutamic acid | [C00624](http://www.genome.jp/dbget-bin/www_bget?cpd:C00624) | [HMDB01138](http://www.hmdb.ca/metabolites/HMDB01138) | 120 | 153.5 | 188.05682 | 13.2 | 237.6  | 1.9  |
| **(M+H)+** | **Annotation** | **KEGG ID** | **HMDB** | **Count/120** | **Avg pm/mg** | ***m/z*** | **MT** | **S/N** | **S/N** |
| C\_0070 | Methionine sulfoxide | [C02989](http://www.genome.jp/dbget-bin/www_bget?cpd:C02989) | [HMDB02005](http://www.hmdb.ca/metabolites/HMDB02005) | 120 | 8 | 166.05368 | 13.7 | 7.7  | 3.1  |
| C\_0101 | SDMA | No ID | [HMDB03334](http://www.hmdb.ca/metabolites/HMDB03334) | 120 | 2.6 | 203.15074 | 8.7 | 7.2  | 1.1  |
| C\_0111 | Cystathionine | [C00542,C02291](http://www.genome.jp/dbget-bin/www_bget?cpd:C00542) | [HMDB00099](http://www.hmdb.ca/metabolites/HMDB00099) | 120 | 586.5 | 223.0756 | 11.3 | 265.7  | 6.6  |
| C\_0152 | Argininosuccinic acid | [C03406](http://www.genome.jp/dbget-bin/www_bget?cpd:C03406) | [HMDB00052](http://www.hmdb.ca/metabolites/HMDB00052) | 120 | 3.5 | 291.13074 | 10.7 | 8.8  | 1.2  |
| C\_0164 | *S*-Adenosylhomocysteine | [C00021](http://www.genome.jp/dbget-bin/www_bget?cpd:C00021) | [HMDB00939](http://www.hmdb.ca/metabolites/HMDB00939) | 120 | 13.9 | 385.1297 | 9.9 | 34.6  | 1.2  |
| C\_0008 | Ala | [C00041,C00133,C01401](http://www.genome.jp/dbget-bin/www_bget?cpd:C00041) | [HMDB00161,HMDB01310](http://www.hmdb.ca/metabolites/HMDB00161) | 120 | 1916.3 | 90.055 | 10.2 | 397.2  | 14.5  |
| C\_0012 | GABA | [C00334](http://www.genome.jp/dbget-bin/www_bget?cpd:C00334) | [HMDB00112](http://www.hmdb.ca/metabolites/HMDB00112) | 120 | 1239 | 104.0709 | 8.6 | 249.8  | 14.9  |
| C\_0014 | Choline | [C00114](http://www.genome.jp/dbget-bin/www_bget?cpd:C00114) | [HMDB00097](http://www.hmdb.ca/metabolites/HMDB00097) | 120 | 495.8 | 104.1073 | 7.6 | 567.5  | 2.6  |
| C\_0029 | Cys | [C00097,C00736,C00793](http://www.genome.jp/dbget-bin/www_bget?cpd:C00097) | [HMDB00574,HMDB03417](http://www.hmdb.ca/metabolites/HMDB00574) | 120 | 201.7 | 122.0272 | 13 | 229.5  | 2.6  |
| C\_0040 | Creatine | [C00300](http://www.genome.jp/dbget-bin/www_bget?cpd:C00300) | [HMDB00064](http://www.hmdb.ca/metabolites/HMDB00064) | 120 | 6494.8 | 132.0769 | 10 | 5611.4  | 3.5  |
| C\_0041 | Ornithine | [C00077,C00515,C01602](http://www.genome.jp/dbget-bin/www_bget?cpd:C00077) | [HMDB00214,HMDB03374](http://www.hmdb.ca/metabolites/HMDB00214) | 120 | 50.8 | 133.0974 | 7.6 | 35.9  | 4.2  |
| C\_0043 | Asp | [C00049,C00402,C16433](http://www.genome.jp/dbget-bin/www_bget?cpd:C00049) | [HMDB00191,HMDB06483](http://www.hmdb.ca/metabolites/HMDB00191) | 120 | 1786.4 | 134.0449 | 13.3 | 391.0  | 13.7  |
| C\_0055 | Spermidine | [C00315](http://www.genome.jp/dbget-bin/www_bget?cpd:C00315) | [HMDB01257](http://www.hmdb.ca/metabolites/HMDB01257) | 120 | 30.8 | 146.1653 | 4.9 | 137.4  | 0.7  |
| C\_0056 | Gln | [C00064,C00303,C00819](http://www.genome.jp/dbget-bin/www_bget?cpd:C00064) | [HMDB00641,HMDB03423](http://www.hmdb.ca/metabolites/HMDB00641) | 120 | 4990.4 | 147.0767 | 12.3 | 1435.4  | 10.4  |
| C\_0058 | Glu | [C00025,C00217,C00302](http://www.genome.jp/dbget-bin/www_bget?cpd:C00025) | [HMDB00148,HMDB03339](http://www.hmdb.ca/metabolites/HMDB00148) | 120 | 8074.9 | 148.0608 | 12.6 | 2890.6  | 8.4  |
| C\_0059 | Met | [C00073,C00855,C01733](http://www.genome.jp/dbget-bin/www_bget?cpd:C00073) | [HMDB00696](http://www.hmdb.ca/metabolites/HMDB00696) | 120 | 218.7 | 150.0587 | 12.3 | 219.9  | 3.0  |
| C\_0076 | Arg | [C00062,C00792](http://www.genome.jp/dbget-bin/www_bget?cpd:C00062) | [HMDB00517,HMDB03416](http://www.hmdb.ca/metabolites/HMDB00517) | 120 | 499.4 | 175.1189 | 7.9 | 597.7  | 2.5  |
| C\_0078 | Citrulline | [C00327](http://www.genome.jp/dbget-bin/www_bget?cpd:C00327) | [HMDB00904](http://www.hmdb.ca/metabolites/HMDB00904) | 120 | 76.1 | 176.1039 | 12.7 | 46.1  | 4.9  |
| C\_0154 | Glutathione (GSSG) divalent | [C00127](http://www.genome.jp/dbget-bin/www_bget?cpd:C00127) | [HMDB03337](http://www.hmdb.ca/metabolites/HMDB03337) | 120 | 165.1 | 307.0841 | 14.1 | 394.1  | 1.3  |
| C\_0001 | Urea\* | C00086 | HMDB00294 | 120 | 0.56\* | 61.04 | 23.6 | 84.1  | 0.02  |
| C\_0005 | Putrescine | [C00134](http://www.genome.jp/dbget-bin/www_bget?cpd:C00134) | [HMDB01414](http://www.hmdb.ca/metabolites/HMDB01414) | 119 | 24.6 | 89.1073 | 5.1 | 15.0  | 4.9  |
| C\_03166 | *N*-Acetylaspartic acid\* | [C01042](http://www.genome.jp/dbget-bin/www_bget?cpd:C01042) | [HMDB00812](http://www.hmdb.ca/metabolites/HMDB00812) | 119 | 6.12 \* | 176.055 | 26.49 | 4502.3  | 0.0  |
| C\_0165 | *S*-Adenosylmethionine | [C00019](http://www.genome.jp/dbget-bin/www_bget?cpd:C00019) | [HMDB01185](http://www.hmdb.ca/metabolites/HMDB01185) | 119 | 8 | 399.1454 | 7.9 | 24.3  | 1.0  |
| C\_0155 | Glutathione (GSH) | [C00051](http://www.genome.jp/dbget-bin/www_bget?cpd:C00051) | [HMDB00125](http://www.hmdb.ca/metabolites/HMDB00125) | 113 | 172.3 | 308.0917 | 15.5 | 302.7  | 1.7  |
| C\_0024 | Betaine | [C00719](http://www.genome.jp/dbget-bin/www_bget?cpd:C00719) | [HMDB00043](http://www.hmdb.ca/metabolites/HMDB00043) | 93 | 124.6 | 118.0865 | 13 | 7.0  | 53.6  |
| C\_0102 | Spermine | [C00750](http://www.genome.jp/dbget-bin/www_bget?cpd:C00750) | [HMDB01256](http://www.hmdb.ca/metabolites/HMDB01256) | 62 | 7.3 | 203.2234 | 4.9 | 8.1  | 2.7  |

\* Indicates that relative measurements were performed for these two metabolites. The values provided represent the average areas of urea and NAA peaks relative to the methionine sulfone internal standard added to the test samples.

\*\* Spermine was dropped from analysis due to above threshold (> 30%) missing values.

S/N; signal:noise

Count/120 denotes the total number of samples in which the metabolite was detected