

Table S2: List of chemicals for preparing the QC, related to “Preparing control samples” section.

| No. | Name | KEGG Number | CAS Number | Company, Catalog # | Solvent for intermediate dilution | Intermediate dilution | Solvent for final dilution | Final conc (stock) mM |
|-----|--------------------------------------|-------------|-------------|--------------------|-----------------------------------|-----------------------|----------------------------|-----------------------|
| 1 | 2-Aminobutyric acid | C02356 | 1492-24-6 | Sigma A1879 | water | 50mM | water | 1 |
| 2 | 2-Ketoglutaric acid | C00026 | 328-50-7 | Sigma 61234 | water | 50mM | water | 1 |
| 3 | 2-Morpholinoethanesulfonic acid | ClS001 | 145224-94-8 | Sigma M8250 | water | 50mM | water | 1 |
| 4 | 3-Hydroxy-D, L-Kynurenine | C02794 | 2147-61-7 | Sigma 78047 | water | 50mM | water | 1 |
| 5 | 4-Aminobutyric acid | C00334 | 56-12-2 | Sigma A2129 | water | 50mM | water | 1 |
| 6 | 4-Hydroxyproline | C01157 | 51-35-4 | Sigma 30681 | water | 50mM | water | 1 |
| 7 | 5-Glutamylcysteine | C00669 | 636-58-8 | Sigma G0903 | water | 50mM | water | 1 |
| 8 | Acetylcarnitine | C02571 | 14992-62-2 | Sigma A1509 | water | 50mM | water | 1 |
| 9 | Acetylcholine | C01996 | 51-84-3 | Sigma A6625 | water | 50mM | water | 1 |
| 10 | Acetic acid | C00417 | 585-84-2 | Sigma A3412 | water | 50mM | water | 1 |
| 11 | Adenine | C00147 | 73-24-5 | Wako 1-79 | 0.5 M HCl | 100mM | water | 1 |
| 12 | Adenosine | C00212 | 58-61-7 | Wako 010-10491 | 1 M NH4OH | 100mM | water | 1 |
| 13 | Adenosine 3',5'-cyclic monophosphate | C00575 | 60-92-4 | Sigma A6885 | water | 50mM | water | 1 |
| 14 | Adenosine monophosphate | C00020 | 61-19-8 | Sigma A1752 | water | 50mM | water | 1 |
| 15 | Adenylylsuccinic acid | C03794 | 19046-78-7 | Sigma A5028 | water | 50mM | water | 1 |
| 16 | Alanine | C00041 | 56-41-7 | Sigma A7627 | water | 50mM | water | 1 |
| 17 | Allantoin | C02348 | 97-59-6 | Sigma 05670 | water | 50mM | water | 1 |
| 18 | Anthranilic Acid | C00108 | 118-92-3 | Sigma 10680 | water | 50mM | water | 1 |
| 19 | Arginine | C00062 | 74-79-3 | Wako 017-04612 | water | 50mM | water | 1 |
| 20 | Argininosuccinic acid | C03406 | 2387-71-5 | Sigma A5707 | water | 50mM | water | 1 |
| 21 | Asparagine | C00152 | 70-47-3 | Sigma A0884 | water | 50mM | water | 1 |
| 22 | Aspartic acid | C00049 | 56-84-8 | Sigma A9256 | 0.5 M HCl | 100mM | water | 1 |
| 23 | Asymmetric dimethylarginine | C03626 | 102783-24-4 | Sigma D4268 | water | 50mM | water | 1 |
| 24 | Carnitine | C00487 | 406-76-8 | Nakarai E1400 | water | 50mM | water | 1 |
| 25 | Carnosine | C00386 | 305-84-0 | Sigma C9625 | water | 50mM | water | 1 |
| 26 | Cholic acid | C00695 | 81-25-4 | Sigma C1254 | water | 50mM | water | 1 |
| 27 | Choline | C00114 | 62-49-7 | Sigma C7017 | water | 50mM | water | 1 |
| 28 | Citicoline | C00307 | 987-78-0 | Sigma 34015 | water | 50mM | water | 1 |
| 29 | Citric acid | C00158 | 77-92-9 | Wako 035-03495 | water | 50mM | water | 1 |
| 30 | Citrulline | C00327 | 372-75-8 | Sigma C7629 | water | 50mM | water | 1 |
| 31 | Creatine | C00300 | 57-00-1 | Sigma C0780 | water | 50mM | water | 1 |
| 32 | Creatinine | C00791 | 60-27-5 | Sigma C4255 | water | 50mM | water | 1 |
| 33 | Cystathionine | C02291 | 56-88-2 | Sigma C7505 | water | 50mM | water | 1 |
| 34 | Cysteamine | C01678 | 60-23-1 | Sigma M9768 | water | 50mM | water | 1 |
| 35 | Cysteine | C00097 | 52-90-4 | Sigma 168149 | water | 50mM | water | 1 |
| 36 | Cystine | C00491 | 56-89-3 | Wako #2706 | 1 M HCl | 100mM | water | 1 |
| 37 | Cytidine | C00475 | 65-46-3 | Wako #035-23231 | water | 50mM | water | 1 |
| 38 | Cytidine 3',5'-cyclic monophosphate | C00941 | 3616-08-8 | Sigma C0985 | water | 50mM | water | 1 |
| 39 | Cytidine monophosphate | C00055 | 63-37-6 | Sigma C1006 | water | 50mM | water | 1 |
| 40 | Cytosine | C00380 | 71-30-7 | Sigma C3506 | 0.1 M HCl | 100mM | water | 1 |
| 41 | Dimethylglycine | C01026 | 1118-68-9 | Wako 350-30981 | water | 50mM | water | 1 |
| 42 | Dopa | C00355 | 59-92-7 | TRC D533751 | 0.5M HCl | 100mM | water | 1 |
| 43 | Dopamine | C03758 | 51-61-6 | Sigma H8502 | water | 50mM | water | 1 |
| 44 | Epinephrine | C00788 | 51-43-4 | Sigma E4250 | 0.5M HCl | 100mM | water | 1 |
| 45 | FAD | C00016 | 146-14-5 | Sigma F6625 | water | 50mM | water | 1 |
| 46 | FMN | C00061 | 146-17-8 | Sigma F2253 | water | 50mM | water | 1 |
| 47 | Fumaric acid | C00122 | 110-17-8 | Wako 069-00652 | ethanol | 50mM | water | 1 |
| 48 | Glutamic acid | C00025 | 56-86-0 | Sigma G1251 | 1 M HCl | 100mM | water | 1 |
| 49 | Glutamine | C00064 | 56-85-9 | Sigma G3126 | water | 50mM | water | 1 |
| 50 | Glutathione | C00051 | 70-18-8 | Wako 077-02011 | water | 50mM | water | 1 |
| 51 | Glycine | C00037 | 56-40-6 | Wako 077-00735 | water | 50mM | water | 1 |
| 52 | Guanine | C00242 | 73-40-5 | Wako 7-109 | 1M HCl | 100mM | water | 1 |
| 53 | Guanosine | C00387 | 118-00-3 | Sigma G6752 | DMSO | 100mM | water | 1 |
| 54 | Guanosine 3',5'-cyclic monophosphate | C00942 | 7665-99-8 | Sigma G6129 | water | 50mM | water | 1 |
| 55 | Guanosine monophosphate | C00144 | 85-32-5 | Sigma G8377 | water | 50mM | water | 1 |
| 56 | Histamine | C00388 | 51-45-6 | Sigma H7125 | water | 50mM | water | 1 |
| 57 | Histidine | C00135 | 71-00-1 | Wako 084-00682 | water | 50mM | water | 1 |
| 58 | Homocysteine | C00155 | 6027-13-0 | Sigma 69453 | water | 50mM | water | 1 |
| 59 | Homocystine | C01817 | 462-10-2 | Sigma H6010 | 0.5M HCl | 100mM | water | 1 |
| 60 | Hypoxanthine | C00262 | 68-94-0 | Sigma H9377 | 1M HCl | 100mM | water | 1 |
| 61 | Inosine | C00294 | 58-63-9 | Sigma I4125 | water | 50mM | water | 1 |
| 62 | Isoctric acid | C00311 | 320-77-4 | Sigma I1252 | water | 50mM | water | 1 |
| 63 | Isoleucine | C00407 | 73-32-5 | Kyowa 552 | water | 50mM | water | 1 |
| 64 | Kynurenic Acid | C01717 | 492-27-3 | Sigma 67667 | 1 M NaOH | 100mM | water | 1 |
| 65 | Kynurenine | C00328 | 2922-83-0 | Sigma K8625 | 0.5M HCl | 100mM | water | 1 |
| 66 | L-Hydroorotic Acid | C00337 | 5988-19-2 | Sigma D7128 | DMSO | 100mM | water | 1 |
| 67 | Lactic acid | C00186 | 79-33-4 | Sigma 252476 | water | 50mM | water | 1 |
| 68 | Leucine | C00123 | 61-90-5 | Wako 124-00852 | water | 50mM | water | 1 |
| 69 | Lysine | C00047 | 56-87-1 | Wako 121-01462 | water | 50mM | water | 1 |
| 70 | Malic acid | C00149 | 97-67-6 | Sigma M0875 | water | 50mM | water | 1 |
| 71 | Methionine | C00073 | 63-68-3 | Sigma M9625 | water | 50mM | water | 1 |
| 72 | Methionine sulfone | ClS002 | 7314-32-1 | Sigma M0751 | water | 50mM | water | 1 |
| 73 | Methionine sulfoxide | C02989 | 3226-65-1 | Sigma M1001 | water | 50mM | water | 1 |
| 74 | NAD | C00003 | 53-84-9 | Sigma N1511 | water | 50mM | water | 1 |
| 75 | Niacinamide | C00153 | 98-92-0 | Sigma N5535 | water | 50mM | water | 1 |
| 76 | Nicotinic acid | C00253 | 59-67-6 | TCI N082 | water | 50mM | water | 1 |
| 77 | Norepinephrine | C00547 | 51-41-2 | Sigma 74480 | water | 50mM | water | 1 |
| 78 | Ophthalmic acid | C21016 | 495-27-2 | Wako H-3145 | water | 50mM | water | 1 |
| 79 | Ornithine | C00077 | 70-26-8 | Sigma O2375 | water | 50mM | water | 1 |
| 80 | Orotic acid | C00295 | 65-86-1 | Sigma O2750 | water | 50mM | water | 1 |
| 81 | Oxidized glutathione | C00127 | 27025-41-8 | Wako 079-03333 | water | 50mM | water | 1 |
| 82 | Pantothenic acid | C00864 | 79-83-4 | Sigma 21210 | water | 50mM | water | 1 |
| 83 | Phenylalanine | C00079 | 63-91-2 | Nakarai 26910 | water | 50mM | water | 1 |
| 84 | Proline | C00148 | 147-85-3 | Nakarai 29001 | water | 50mM | water | 1 |
| 85 | Putrescine | C00134 | 110-60-1 | Sigma 51799 | water | 50mM | water | 1 |
| 86 | Pyruvic acid | C00022 | 127-17-3 | Sigma 107360 | water | 50mM | water | 1 |
| 87 | S-Adenosylhomocysteine | C00021 | 979-92-0 | Sigma A9384 | 1 M HCl | 100mM | water | 1 |
| 88 | S-Adenosylmethionine | C00019 | 29908-03-0 | NEB B9003S | water | 50mM | water | 1 |
| 89 | Serine | C00065 | 56-45-1 | Wako 199-00402 | water | 50mM | water | 1 |
| 90 | Serotonin | C00780 | 50-67-9 | Sigma H9523 | water | 50mM | water | 1 |
| 91 | Spermidine | C00315 | 124-20-9 | Sigma 49761 | water | 50mM | water | 1 |
| 92 | Spermine | C00750 | 71-44-3 | Sigma 55513 | water | 50mM | water | 1 |
| 93 | Succinic acid | C00042 | 110-15-6 | Sigma S3674 | water | 50mM | water | 1 |
| 94 | Symmetric dimethylarginine | C03626 | 102783-24-4 | Sigma D0390 | water | 50mM | water | 1 |
| 95 | Taurocholic acid | C05122 | 81-24-3 | Sigma 86339 | water | 50mM | water | 1 |
| 96 | Threonine | C00188 | 72-19-5 | Wako 204-01322 | water | 50mM | water | 1 |
| 97 | Thymidine | C00214 | 50-89-5 | Sigma T9250 | water | 50mM | water | 1 |
| 98 | Thymidine monophosphate | C00364 | 365-07-1 | Sigma T7004 | water | 50mM | water | 1 |
| 99 | Thymine | C00178 | 65-71-4 | Wako 20-139 | water | 50mM | water | 1 |
| 100 | Tryptophan | C00078 | 73-22-3 | Wako 204-03382 | 0.5M HCl | 100mM | water | 1 |
| 101 | Tyrosine | C00082 | 60-18-4 | Sigma T3754 | 0.5M HCl | 100mM | water | 1 |
| 102 | Uracil | C00106 | 66-22-8 | Wako 212-00062 | water | 50mM | water | 1 |
| 103 | Uric acid | C00366 | 69-93-2 | Sigma U2825 | 1 M NaOH | 100mM | water | 1 |
| 104 | Uridine | C00299 | 58-96-8 | Sigma U3750 | water | 50mM | water | 1 |
| 105 | Valine | C00183 | 72-18-4 | Wako 226-00083 | water | 50mM | water | 1 |
| 106 | Xanthine | C00385 | 69-89-6 | Sigma X0626 | 1 M NaOH | 100mM | water | 1 |

Table S3: Analysis of the Blank, related to “Systems performance check” section.

| Compound Name | Blank | |
|--------------------------------------|----------------------|-------|
| | Average 3 replicates | SD |
| 2-Aminobutyric acid | | |
| 2-Ketoglutaric acid | | |
| 3-Hydroxy-D L-Kynurenine | | |
| 4-Aminobutyric acid | | |
| 4-Hydroxyproline | | |
| 5-Glutamylcysteine | | |
| Acetylcamitine | | |
| Acetylcholine | | |
| Aconitic acid | | |
| Adenine | | |
| Adenosine 3',5'-cyclic monophosphate | | |
| Adenosine monophosphate | | |
| Adenosine | | |
| Adenylsuccinic acid | | |
| Alanine | | |
| Allantoin | | |
| Anthranilic Acid | | |
| Arginine | | |
| Argininosuccinic acid | | |
| Asparagine | | |
| Aspartic acid | 0.005 | 0.001 |
| Asymmetric dimethylarginine | | |
| Camitine | | |
| Camosine | | |
| Cholic Acid (CA) | | |
| Choline | 0.528 | 0.042 |
| Citicoline | | |
| Citric Acid | | |
| Citrulline | | |
| Creatine | | |
| Creatinine | | |
| Cystathionine | | |
| Cysteamine | | |
| Cysteine | | |
| Cystine | | |
| Cytidine 3',5'-cyclic monophosphate | | |
| Cytidine monophosphate | | |
| Cytidine | | |
| Cytosine | | |
| Dimethylglycine | | |
| Dopa | | |
| Dopamine | | |
| FAD | | |
| Epinephrine | | |
| FMN | | |
| Fumaric Acid | | |
| Glutamic acid | | |
| Glutamine | | |
| Glutathione oxidazed | | |
| Glutathione reduced | | |
| Glycine | 0.030 | 0.001 |
| Guanine | | |
| Guanosine 3',5'-cyclic monophosphate | | |
| Guanosine monophosphate | | |
| Guanosine | 0.007 | 0.001 |
| Histamine | | |
| Histidine | | |
| Homocysteine | | |
| Homocystine | | |
| Hypoxanthine | | |
| Inosine | | |
| Isocitric Acid | | |
| Isoleucine | | |
| Kynurenic Acid | | |
| Kynurenine | | |
| Lactic Acid | 0.028 | 0.001 |
| Leucine | | |
| L-Hydrorootic Acid | | |
| Lysine | | |
| Malic Acid | | |
| Methionine sulfone | | |
| Methionine sulfoxide | | |
| Methionine | | |
| NAD | | |
| Niacinamide | | |
| Nicotinic acid | | |
| Norepinephrine | | |
| Ophthalmic acid | | |
| Omitine | | |
| Orotic Acid Pos | | |
| Pantothenic acid | | |
| Phenylalanine | | |
| Picolinic Acid | | |
| Proline | | |
| Putrescine | 5.165 | 0.720 |
| Pyruvic acid | | |
| Ribitol | | |
| S-Adenosylhomocysteine | | |
| S-Adenosylmethionine | | |
| Sarcosine | | |
| Serine | | |
| Serotonin | | |
| Spermidine | | |
| Spermine | | |
| Succinic acid | 0.007 | 0.001 |
| Symmetric dimethylarginine | | |
| Taurine | | |
| Taurocholic acid | | |
| Threonine | 0.003 | 0.001 |
| Thymidine monophosphate | | |
| Thymidine | 0.001 | 0.000 |
| Thymine | | |
| Tryptophan | | |
| Tyrosine | | |
| Uracil | | |
| Uric acid | | |
| Uridine | | |
| Valine | | |
| Xanthine | | |

Table S4: Analysis of the QC, related to "Systems performance check" section.

| Compound Name | QC-Rep1 | | QC-Rep2 | | QC-Rep3 | | JPN mix | |
|--------------------------------------|-------------|------------|------------|------------|-------------|------------|------------|------------|
| | Area | Area/ISTD | Area | Area/ISTD | Area | Area/ISTD | Average | SD |
| 2-Aminobutyric acid | 150340.029 | 0.16919431 | 155630.858 | 0.17795299 | 165246.948 | 0.17250208 | 0.17321646 | 0.00442283 |
| 2-Morpholinoethansulfonic Acid | 888564.34 | 1 | 874561.63 | 1 | 957941.77 | 1 | 1 | 0 |
| 3-Hydroxy-D L-Kynurenine | 416473.591 | 0.46870392 | 417581.344 | 0.47747504 | 412376.463 | 0.43048176 | 0.45888691 | 0.02498744 |
| 4-Aminobutyric acid | 290945.988 | 0.32743379 | 346787.777 | 0.39652755 | 333450.633 | 0.34809071 | 0.35735068 | 0.03546544 |
| 4-Hydroxyproline | 386549.664 | 0.43502721 | 390117.346 | 0.44607188 | 415673.948 | 0.43392402 | 0.43834104 | 0.00671779 |
| 5-Glutamylcysteine | 8954.70609 | 0.01007772 | 14267.529 | 0.01631392 | 10176.7792 | 0.01062359 | 0.01233841 | 0.00345369 |
| Acetylcamitine | 1865675.4 | 20.996516 | 19247991 | 22.0087303 | 18678316.3 | 19.4983838 | 20.8345434 | 1.26298703 |
| Acetylcholine | 2644.04421 | 0.00297564 | 2772.84077 | 0.00317055 | 2521.01403 | 0.0026317 | 0.00292596 | 0.00027284 |
| Aconitic acid | 127702.343 | 0.14371761 | 114446.063 | 0.13086106 | 101382.161 | 0.10583332 | 0.126804 | 0.01926524 |
| Adenine | 169639.899 | 0.19091459 | 159932.71 | 0.18287186 | 127565.805 | 0.13316655 | 0.16898433 | 0.03127869 |
| Adenosine 3',5'-cyclic monophosphate | 2254104.33 | 2.5367936 | 2200275.28 | 2.51586075 | 2313153.61 | 2.41471212 | 2.48912216 | 0.06528542 |
| Adenosine monophosphate | 6803569.83 | 7.6568117 | 6835403.47 | 7.81580537 | 6127015.93 | 6.39602125 | 7.28954611 | 0.77788801 |
| Adenosine | 2126390.92 | 2.39306348 | 1777615.16 | 2.03257849 | 1227016.06 | 1.28088794 | 1.90217664 | 0.56743907 |
| Adenylsuccinic acid | 235184.445 | 0.26467914 | 239162.995 | 0.27346614 | 216950.06 | 0.22647521 | 0.2548735 | 0.02498299 |
| Alanine | 136497.252 | 0.1536155 | 130580.496 | 0.14930966 | 143848.243 | 0.15016387 | 0.15102967 | 0.00227975 |
| Allantoin | 5341.33572 | 0.0060112 | 4480.31589 | 0.00512293 | 5115.79968 | 0.00534041 | 0.00549151 | 0.00046301 |
| Anthrancilic Acid | 205415.207 | 0.23117651 | 201073.84 | 0.22991386 | 199648.595 | 0.20841412 | 0.22316817 | 0.01279296 |
| Arginine | 3477525.52 | 3.91364515 | 3058049.15 | 3.49666513 | 3417831.35 | 3.5678905 | 3.65940026 | 0.22304397 |
| Argininosuccinic acid | 9525.24194 | 0.01071981 | 7946.9333 | 0.00908676 | 8287.18988 | 0.00865104 | 0.00948587 | 0.00190961 |
| Asparagine | 130133.35 | 0.14645349 | 127814.842 | 0.14614732 | 131507.375 | 0.13728118 | 0.143294 | 0.00520995 |
| Aspartic acid | 466240.11 | 0.52471171 | 456217.342 | 0.52165259 | 482132.388 | 0.50330031 | 0.51655487 | 0.01158025 |
| Asymmetric dimethylarginine | 26048.2839 | 0.02931502 | 18187.5251 | 0.02079616 | 30234.3044 | 0.03156174 | 0.02722431 | 0.00567915 |
| Camitine | 3723680.26 | 4.19067038 | 3623170.11 | 4.14284139 | 2212212.39 | 2.3093391 | 3.54761696 | 1.0726467 |
| Camosine | 1619076 | 1.82212579 | 1813476.96 | 2.07358396 | 2047728.07 | 2.13763313 | 2.01111429 | 0.1667725 |
| Cholic Acid (CA) | 5344.18265 | 0.0060144 | 5577.32153 | 0.00637728 | 5623.23949 | 0.00587013 | 0.00608727 | 0.00026131 |
| Choline | 5480851.85 | 6.16821046 | 5125977.72 | 5.86119669 | 5808354.79 | 6.06336936 | 6.0309225 | 0.15605709 |
| Citicoline | 223969.934 | 0.25205821 | 212339.09 | 0.24279488 | 204189.982 | 0.25073547 | 0.24852952 | 0.00501018 |
| Citric Acid | 84716.8141 | 0.09534123 | 89355.3969 | 0.10217164 | 45322.1275 | 0.04731199 | 0.08160828 | 0.02989717 |
| Citrulline | 786071.243 | 0.88465315 | 805305.42 | 0.92081037 | 872197.388 | 0.91049103 | 0.90531818 | 0.01862538 |
| Creatine | 497877.619 | 0.5603169 | 797832.122 | 0.91226518 | 510463.937 | 0.53287575 | 0.66848594 | 0.21156439 |
| Creatinine | 6328316.51 | 7.12195643 | 6204505.54 | 7.09441776 | 5722006.21 | 5.97322966 | 6.72986795 | 0.65541263 |
| Cystathionine | 2529778.15 | 2.84703993 | 2426578.62 | 2.77462278 | 2568831.19 | 2.68107234 | 2.76757835 | 0.08320774 |
| Cysteamine | 9653.08681 | 0.01086369 | 24354.7284 | 0.02784793 | 31715.7481 | 0.03310822 | 0.02393995 | 0.01162579 |
| Cysteine | 9788.77045 | 0.01101639 | 9718.95817 | 0.01111295 | 9794.36827 | 0.01022439 | 0.01078458 | 0.00048753 |
| Cystine | 1657385.56 | 1.86523978 | 1596413.31 | 1.82538686 | 1707403.05 | 1.78236621 | 1.82433095 | 0.04144687 |
| Cytidine 3',5'-cyclic monophosphate | 3570274.22 | 4.01802555 | 3487305.17 | 3.98748933 | 3564752.35 | 3.72126204 | 3.90892564 | 0.16323705 |
| Cytidine monophosphate | 2879414.7 | 3.24052471 | 2746095.3 | 3.13996774 | 2951324.48 | 3.08090174 | 3.15379807 | 0.08070521 |
| Cytidine | 3648625.01 | 4.10620238 | 2920977.38 | 3.33993315 | 2395367.79 | 2.5005359 | 3.31555715 | 0.80311074 |
| Cytosine | 1667056.88 | 1.87612399 | 982174.861 | 1.1230482 | 780683.491 | 0.81495923 | 1.27137714 | 0.54591095 |
| Dimethylglycine | 227018.483 | 0.25548908 | 202032.912 | 0.23101049 | 211832.21 | 0.22113266 | 0.23587741 | 0.01768774 |
| Dopa | 21711790.14 | 2.44415631 | 2267160.98 | 2.59233987 | 20414053.39 | 2.52004189 | 2.51884602 | 0.07409902 |
| Dopamine | 2028666.47 | 2.28308337 | 1999720.69 | 2.28654063 | 2008794.41 | 2.09699009 | 2.2222047 | 0.10845281 |
| Epinephrine | 2761353.88 | 3.10765777 | 2537523.39 | 2.90148037 | 2398780.98 | 2.50409895 | 2.8377457 | 0.30678559 |
| FMN | 127850.907 | 0.1438848 | 121755.087 | 0.13921842 | 128105.83 | 0.13373029 | 0.1389445 | 0.0050828 |
| Fumaric Acid | 10785.0253 | 0.01213759 | 10197.182 | 0.01165976 | 10620.4376 | 0.01108673 | 0.01162802 | 0.00052615 |
| Glutamic acid | 788716.9231 | 0.88763063 | 763948.943 | 0.87352214 | 730590.827 | 0.76266726 | 0.84127334 | 0.06843938 |
| Glutamine | 92822.8343 | 0.10446383 | 91221.9304 | 0.10430589 | 91517.7116 | 0.09553578 | 0.10143517 | 0.00510963 |
| Glutathione oxidized | 196710.996 | 0.22137969 | 209285.256 | 0.23930304 | 217460.442 | 0.227008 | 0.22923024 | 0.00916599 |
| Glutathione reduced | 35525.1677 | 0.03998041 | 36774.6313 | 0.04204922 | 37099.8547 | 0.03872872 | 0.04025278 | 0.00167692 |
| Glycine | 70749.431 | 0.07962218 | 72908.0684 | 0.08336527 | 76314.4721 | 0.07966504 | 0.08088417 | 0.00214881 |
| Guanine | 15135.5472 | 0.01703371 | 15595.5424 | 0.01783241 | 25831.0418 | 0.02696515 | 0.02601042 | 0.00551782 |
| Guanosine 3',5'-cyclic monophosphate | 824264.517 | 0.92763628 | 808948.275 | 0.92497572 | 875439.217 | 0.91387519 | 0.9221624 | 0.00729918 |
| Guanosine monophosphate | 530166.592 | 0.59665527 | 509905.951 | 0.58304176 | 582464.686 | 0.60803767 | 0.59591157 | 0.01251454 |
| Guanosine | 4702905.84 | 5.29270153 | 4643539.68 | 5.30956257 | 4387051.91 | 4.57966448 | 5.06064286 | 0.4166248 |
| Histamine | 1146555.32 | 1.29034586 | 1107472.34 | 1.2663171 | 1333470.13 | 1.39201585 | 1.31622627 | 0.06672624 |
| Histidine | 388288.09 | 0.43698461 | 359364.192 | 0.41090797 | 3983922.78 | 4.15883605 | 4.21258621 | 0.13844356 |
| Homocysteine | 7469.90802 | 0.00840672 | 40691.187 | 0.04652752 | 50879.7822 | 0.05311363 | 0.03601596 | 0.02413601 |
| Homocystine | 1031407.92 | 1.16075773 | 1047319.53 | 1.19753657 | 1182092.47 | 1.23399198 | 1.19742876 | 0.03661725 |
| Hypoxanthine | 93501.225 | 1.05227296 | 932483.579 | 1.0662297 | 672343.977 | 0.7018631 | 0.94012192 | 0.20645616 |
| Inosine | 3190015.6 | 3.59007835 | 3134200.29 | 3.58373863 | 3218241.88 | 3.3595381 | 3.51111836 | 0.13131062 |
| Isoelectric Acid | 30756.396 | 0.03461358 | 28843.4283 | 0.03298044 | 31705.6314 | 0.03309766 | 0.0335639 | 0.00091094 |
| Isoleucine | 3252523.32 | 3.66042523 | 3210505.57 | 3.67098838 | 3321394.11 | 3.46721921 | 3.59954427 | 0.11471851 |
| Kynurenic acid | 981.49551 | 0.00110459 | 954.823483 | 0.00109177 | 1043.83789 | 0.00108967 | 0.00109534 | 8.074E-06 |
| Kynurenine | 254155.745 | 0.28602965 | 287685.247 | 0.32894794 | 287601.991 | 0.30022909 | 0.30506889 | 0.02186465 |
| Lactic Acid | 7125.83872 | 0.00812078 | 7142.75554 | 0.00816724 | 9426.28561 | 0.00984014 | 0.00870939 | 0.00097954 |
| Leucine | 3503174.41 | 3.94251069 | 3483839.84 | 3.98352698 | 3541492.02 | 3.69698047 | 3.87433938 | 0.15496039 |
| L-Hydroxotrotic Acid | 14260.6538 | 0.0160491 | 11693.664 | 0.01337089 | 17437.688 | 0.01820329 | 0.01587442 | 0.00242093 |
| Lysine | 1391136.3 | 1.56559997 | 1328997.15 | 1.51961521 | 1431696.98 | 1.49455533 | 1.52659017 | 0.03603224 |
| Malic Acid | 21905.3682 | 0.02465254 | 20161.3466 | 0.02035309 | 23362.9964 | 0.02438874 | 0.02403146 | 0.0008575 |
| Methionine sulfone | 27476.0028 | 0.03092179 | 23821.5084 | 0.02723823 | 27545.0639 | 0.02875442 | 0.02897148 | 0.00185135 |
| Methionine sulfoxide | 872830.288 | 0.98229273 | 1011319.41 | 1.15637295 | 913925.584 | 0.95405129 | 1.03090566 | 0.10957156 |
| Methionine | 1933.69246 | 0.0021762 | 1970.45671 | 0.00225308 | 1600.85035 | 0.00167114 | 0.00203347 | 0.00031614 |
| NAD | 180343.467 | 0.20296051 | 182066.549 | 0.20818035 | 214297.521 | 0.22370621 | 0.21161569 | 0.01079107 |
| Niacinamide | 3982546.98 | 4.48200181 | 3802939.28 | 4.34839486 | 3242401.02 | 3.38475794 | 4.0717182 | 0.59866393 |
| Nicotinic acid | 3243391.61 | 3.65014829 | 2690695.41 | 3.07662185 | 1852339.93 | 1.93366652 | 2.88681222 | 0.87384106 |
| Ophthalmic acid | 111529.39 | 1.25512498 | 1087767.19 | 1.24378563 | 1055161.2 | 1.10148783 | 1.20013281 | 0.085617 |
| Omitine | 789905.241 | 0.88896797 | 733731.754 | 0.8389709 | 800376.96 | 0.83551734 | 0.8544854 | 0.02991266 |
| Orotic Acid Pos | 255291.26 | 0.28730757 | 251150.054 | 0.28717251 | 263181.494 | 0.27473642 | 0.28307217 | 0.00721928 |
| Pantothenic acid | 775981.114 | 0.87329761 | 736596.739 | 0.84224681 | 708352.216 | 0.73945227 | 0.81833223 | 0.07005408 |
| Phenylalanine | 3230492.54 | 3.63563154 | 3211604.05 | 3.67224441 | 3195445.22 | 3.33574056 | 3.54787217 | 0.18462121 |
| Picolinic Acid | 3148631.04 | 3.54350371 | 3480483.47 | 3.9796892 | 3111352.48 | 3.24795574 | 3.59038289 | 0.36811236 |
| Proline | 2784649.57 | 3.133875 | 2770823.57 | 3.16824279 | 3052168.9 | 3.18617372 | 3.16276384 | 0.02657637 |
| Putrescine | 93827.9191 | 0.1059496 | 97215.856 | 0.11115953 | 114786.131 | 0.11982579 | 0.11219343 | 0.00717153 |
| S-Adenosylhomocysteine | 516187.999 | 0.5809236 | 482545.766 | 0.5517573 | 384956.161 | 0.40185758 | 0.51151283 | 0.09607744 |
| S-Adenosylmethionine | 1108476.5 | 1.24749154 | 1257892.19 | 1.43831167 | 196306 | | | |

Table S6: Absolute quantification, related to “Basic data analysis” section.

| Uncorrected | HT29 Ctrl 1 | HT29 Ctrl 2 | HT29 Ctrl 3 | HT29 Ctrl 4 | HT29 Ctrl 5 | Met 10mM 1 | Met 10mM 2 | Met 10mM 3 | Met 10mM 4 | Met 10mM 5 | Met 10mM 6 |
|--------------------------------|-------------|-------------|-------------|-------------|-------------|------------|------------|------------|------------|------------|-------------|
| Compound Name | Area | Area | Area | Area | Area | Area | Area | Area | Area | Area | Area |
| 2-Morpholinoethansulfonic Acid | 295073.12 | 248132.62 | 209232.36 | 302957.98 | 211807.71 | 466792.9 | 452862.37 | 400524.53 | 458171.03 | 443308.52 | 521175.5835 |
| 4-Aminobutyric acid | 860262.423 | 933547.79 | 841638.645 | 952086.577 | 959341.184 | 62467.5009 | 55582.099 | 48883.0699 | 59977.223 | 59245.9859 | 54019.88729 |
| Glutamine | 51937.7803 | 46106.4544 | 44745.9871 | 45507.01 | 43488.9601 | 102278.494 | 46516.7256 | 65590.3006 | 79145.6457 | 75659.4364 | 41280.31657 |
| Tryptophan | 554144.172 | 570531.451 | 501869.129 | 608669.808 | 644947.587 | 467055.267 | 577361.316 | 502435.63 | 462233.088 | 439092.52 | 604016.4963 |

| Corrected | HT29 Ctrl | | HT29 Met | |
|---------------------|-----------|------------|-----------|------------|
| Compound Name | Average | SD | Average | SD |
| 4-Aminobutyric acid | 714465.72 | 127130.991 | 31128.257 | 2664.72553 |
| Glutamine | 12593.238 | 1585.39664 | 12473.522 | 3878.97126 |
| Tryptophan | 103702.47 | 19956.8624 | 60531.983 | 6952.36786 |

| Correction | 1 | 1.18917506 | 1.41026521 | 0.97397377 | 1.39311793 | 0.63212856 | 0.65157351 | 0.73671674 | 0.64402397 | 0.66561573 | 0.566168358 |
|------------|---|------------|------------|------------|------------|------------|------------|------------|------------|------------|-------------|
|------------|---|------------|------------|------------|------------|------------|------------|------------|------------|------------|-------------|

| Corrected | HT29 Ctrl 1 | HT29 Ctrl 2 | HT29 Ctrl 3 | HT29 Ctrl 4 | HT29 Ctrl 5 | Met 10mM 1 | Met 10mM 2 | Met 10mM 3 | Met 10mM 4 | Met 10mM 5 | Met 10mM 6 |
|--------------------------------|-------------|-------------|-------------|-------------|-------------|------------|------------|------------|------------|------------|-------------|
| Compound Name | Area | Area | Area | Area | Area | Area | Area | Area | Area | Area | Area |
| 2-Morpholinoethansulfonic Acid | 295073.12 | 295073.12 | 295073.12 | 295073.12 | 295073.12 | 295073.12 | 295073.12 | 295073.12 | 295073.12 | 295073.12 | 295073.1241 |
| 4-Aminobutyric acid | 860262.42 | 1110151.7 | 1186933.7 | 927307.35 | 1336475.4 | 39487.491 | 36215.823 | 36012.976 | 38626.769 | 39435.06 | 30584.35086 |
| Glutamine | 51937.78 | 54828.646 | 63103.709 | 44322.634 | 60585.25 | 64653.157 | 30309.066 | 48321.472 | 50971.693 | 50360.111 | 23371.60903 |
| Tryptophan | 554144.17 | 678461.77 | 707768.57 | 592828.43 | 898488.05 | 295238.97 | 376193.34 | 370152.74 | 297689.19 | 292266.89 | 341975.0276 |

| Corrected | HT29 Ctrl 1 | HT29 Ctrl 2 | HT29 Ctrl 3 | HT29 Ctrl 4 | HT29 Ctrl 5 | Met 10mM 1 | Met 10mM 2 | Met 10mM 3 | Met 10mM 4 | Met 10mM 5 | Met 10mM 6 |
|---------------------|-------------|-------------|-------------|-------------|-------------|------------|------------|------------|------------|------------|-------------|
| Compound Name | Conc. (nM) | Conc. (nM) | Conc. (nM) | Conc. (nM) | Conc. (nM) | Conc. (nM) | Conc. (nM) | Conc. (nM) | Conc. (nM) | Conc. (nM) | Conc. (nM) |
| 4-Aminobutyric acid | 567253.44 | 731506.74 | 781975.84 | 611322.35 | 880270.22 | 33305.574 | 30724.996 | 30564.998 | 32626.666 | 33264.218 | 26283.08809 |
| Glutamine | 11948.496 | 12566.114 | 14334.038 | 10321.56 | 13795.983 | 17598.084 | 8793.1613 | 13411.069 | 14090.516 | 13933.722 | 7014.579574 |
| Tryptophan | 84004.173 | 102528.8 | 106895.82 | 89768.532 | 135315.01 | 54509.507 | 68985.164 | 67905.029 | 54947.636 | 53978.061 | 62866.50067 |

| | M | B | Dilution Factor |
|---------------------|------------|------------|-----------------|
| 4-Aminobutyric acid | 78.068282 | 2737.47175 | HT29Ctrl 50 |
| Glutamine | 234.033343 | 3989.14942 | HT29Met 60 |
| Tryptophan | 335.546902 | 9602.63134 | |

