Supplementary Information (SI) for Food & Function.
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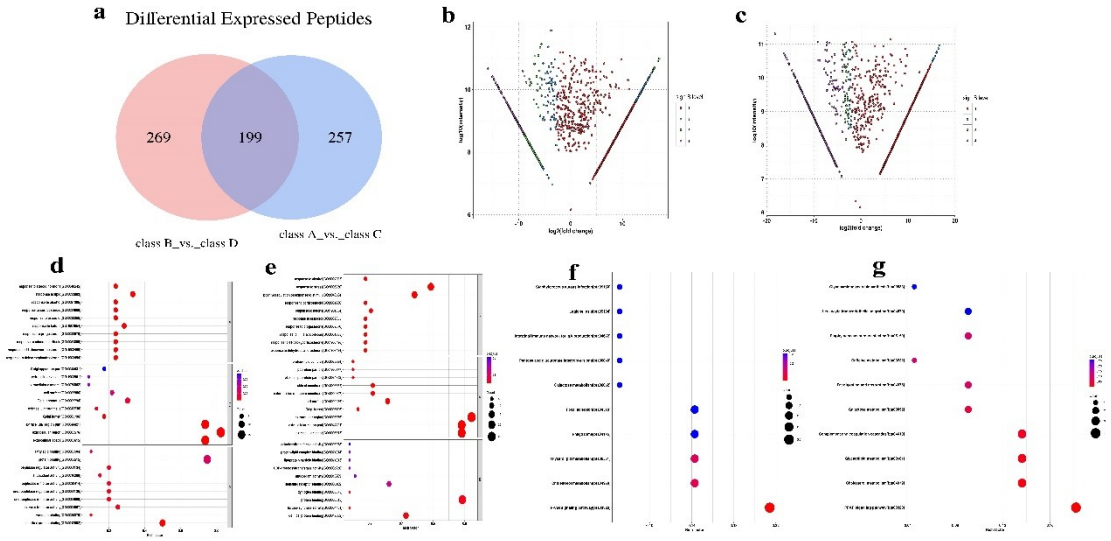
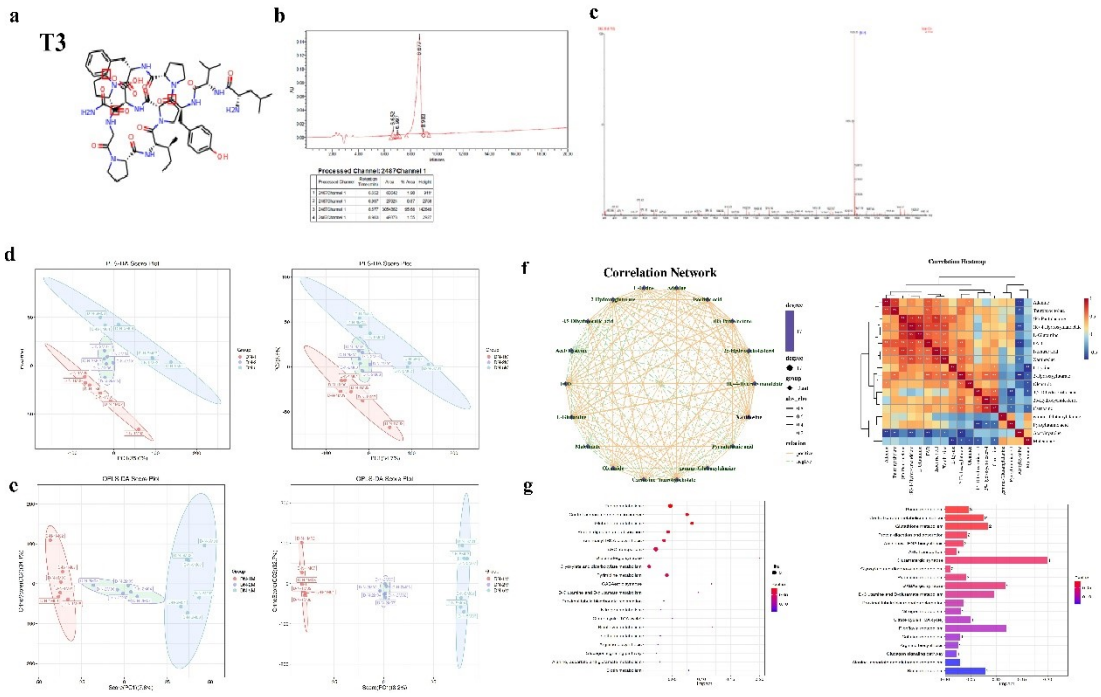
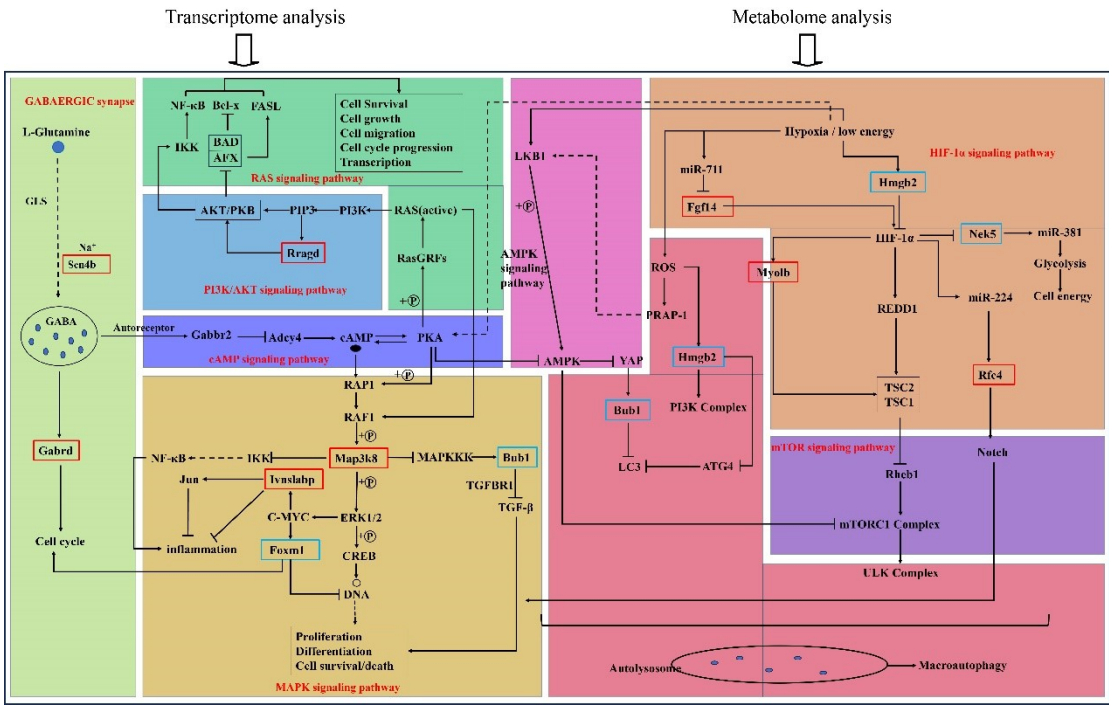



Supplementary Figure. 1 Screening of differential peptides (**a**). Visual analysis of the differential peptides from class A vs class C (**b**) and class B vs class D (**c**). Functional enrichment analysis of the differential peptides from class A vs class C (**d**) and class B vs class D (**e**). KEGG pathway enrichment analysis of the differential peptides from class A vs class C (**f**) and class B vs class D (**g**). class A: peptides of hydrolysate $N_A$ (where obtained from 3100 m sea level); class C: enzymatic hydrolysate of $N_A$; class B: peptides of hydrolysate $N_C$ (where obtained from 4975 m sea level); class D: enzymatic hydrolysate of $N_C$.




Supplementary Figure. 2 Metabolomic differences analysis of hypoxic mice after T3 treatment. **a-c**: Structure of T3 (**a**) and reverse high-performance liquid chromatography was used to determine the purity of T3 (**b, c**). **d** PLS-DA analyzed the metabolites of brain tissues in the brain tissues of BALB/C male mice. **e** OPLS-DA analyzed the metabolites in the brain tissues of BALB/C male mice. Correlation analysis (**f**) and KEGG pathway analysis (**g**) among difference metabolites in the brain tissues of BALB/C male mice after T3 treatments. DN-1M: normoxic saline group (Con); DN-2M: hypoxic saline group (Q-Con); DN-5M: milk residue peptide T3 at medium dose group (T3-50 mg/ kg. $d^{-1}$).




Supplementary figure. 3 Key signaling pathways involved in T3 improved hypoxia induced brain injury in BALB/C male mice (GABAERGIC synthesis and RAS signaling pathway, cAMP signaling pathway, MAPK signaling pathway, HIF-1α signaling pathway, mTOR signaling pathway). Expression profiles of DEMs and CDEGs from brain in BALB/C male mice under different treats. Red border indicates up-regulation, while blue border indicates down-regulation.

Supplementary Table. 1 Peptide Ranker activity scores of yak milk residues

| Code | Gene | Description（protain） | sequence | Mass | PeptideRanker |
|---|---|---|---|---|---|
| T1 | CSN2 | Beta-casein | YPFPGPIPN | 1000.5018 | 0.818687 |
| T2 | CSN2 | Beta-casein | PVVVPPFLQPEVMGVSK | 1822.0063 | 0.513702 |
| T3 | CSN2 | Beta-casein | LVYPFPGPIPN | 1212.6543 | 0.646746 |
| T4 | PIGR | Polymeric immunoglobulin receptor | SPIFGPEEVTSVEGR | 1602.789 | 0.376966 |
| T5 | CSN1S1 | Alpha-S1-casein | QGLPQEVLNE | 1125.5666 | 0.128108 |
| T6 | PLIN2 | Perilipin-2 | LVDQYLPLTKDELEK | 1802.9666 | 0.117669 |
| T7 | CSN1S1 | Alpha-S1-casein | RPKHPIKHQGLPQEVLN | 2119.1651 | 0.459489 |
| T8 | CSN1S1 | Alpha-S1-casein | RPKHPIKHQGLPQ | 1534.8845 | 0.389209 |
| T9 | PIGR | Polymeric immunoglobulin receptor | KSPIFGPEEVTSVEGR | 1730.8839 | 0.37051 |
| T10 | CSN1S1 | Alpha-S1-casein | KHPIKHQGLPQEVLNE | 1866.0112 | 0.221354 |
| T11 | CSN1S1 | Alpha-S1-casein | IKHQGLPQEVLNE | 1503.8045 | 0.141373 |
| T12 | CSN1S1 | Alpha-S1-casein | HQGLPQEVLNENL | 1489.7525 | 0.280315 |
| T13 | CSN1S1 | Alpha-S1-casein | HQGLPQEVLNEN | 1376.6684 | 0.133223 |
| T14 | CSN1S1 | Alpha-S1-casein | HQGLPQEVLNE | 1262.6255 | 0.121401 |
| T15 | CSN1S1 | Alpha-S1-casein | HQGLPQEVL | 1019.54 | 0.226194 |
| T16 | CSN1S1 | Alpha-S1-casein | HPIKHQGLPQEVLNENL | 1965.0432 | 0.356735 |
| T17 | CSN1S1 | Alpha-S1-casein | HPIKHQGLPQEVLNEN | 1851.9591 | 0.202096 |
| T18 | CSN1S1 | Alpha-S1-casein | HPIKHQGLPQEVLNE | 1737.9162 | 0.185815 |
| T19 | CSN1S1 | Alpha-S1-casein | HPIKHQGLPQEVL | 1494.8307 | 0.262609 |

Supplementary Table. 2 ADMET absorption, metabolism, toxicity and sensitization of T1, T2 and T3

| Classfications | T1 | | T2 | | T3 | |
|---|---|---|---|---|---|---|
| Sensitization | NON-ALLERGEN | | ALLERGEN | | NON-ALLERGEN | |
| ADMET predicted profile--classifications | Value | Probaility | Value | Probaility | Value | Probaility |
| Human Intestinal Absorption | + | 0.7205 | + | 0.5961 | + | 0.75 |
| Caco-2 | - | 0.8654 | - | 0.8609 | - | 0.8677 |
| Blood Brain Barrier | - | 0.9 | - | 0.85 | - | 0.925 |
| Human oral bioavailability | - | 0.6143 | - | 0.6286 | - | 0.6429 |
| Subcellular localzation | Mitochondria | 0.539 | Lysosomes | 0.5651 | Mitochondria | 0.5155 |
| OATP2B1 inhibitior | - | 0.8585 | - | 1 | - | 0.8589 |
| OATP1B1 inhibitior | + | 0.8457 | + | 0.8234 | + | 0.8447 |
| OATP1B3 inhibitior | + | 0.9368 | + | 0.9276 | + | 0.9355 |
| MATE1 inhibitior | - | 0.98 | - | 0.9 | - | 0.98 |
| OCT2 inhibitior | - | 0.775 | - | 0.925 | - | 0.75 |
| BSEP inhibitior | + | 0.9205 | + | 0.9716 | + | 0.9489 |
| P-glycoprotein inhibitior | + | 0.7465 | + | 0.7418 | + | 0.7431 |
| P-glycoprotein substrate | + | 0.724 | + | 0.8735 | + | 0.8142 |
| CYP3A4 substrate | + | 0.6909 | + | 0.7511 | + | 0.7191 |
| CYP2C9 substrate | - | 0.7983 | - | 0.8056 | - | 0.7983 |
| CYP2D6 substrate | - | 0.8083 | - | 0.8215 | - | 0.8083 |
| CYP3A4 inhibition | - | 0.8405 | - | 0.9538 | - | 0.6745 |
| CYP2C9 inhibition | - | 0.8738 | - | 0.9197 | - | 0.8572 |
| CYP2C19 inhibition | - | 0.7896 | - | 0.8602 | - | 0.7923 |
| CYP2D6 inhibition | - | 0.8893 | - | 0.925 | - | 0.8916 |
| CYP1A2 inhibition | - | 0.9435 | - | 0.8987 | - | 0.9461 |
| CYP inhibitory promiscuity | - | 0.8758 | - | 0.9884 | - | 0.8597 |
| UGT catelyzed | - | 0.5 | + | 0.7 | - | 0.6 |
| Carcinogenicity (binary) | - | 0.82 | - | 0.8 | - | 0.82 |
| Carcinogenicity (trinary) | Non-required | 0.6427 | Non-required | 0.6565 | Non-required | 0.6304 |
| Eye corrosion | - | 0.9914 | - | 0.9873 | - | 0.9903 |
| Eye irritation | - | 0.9001 | - | 0.8954 | - | 0.8968 |
| Ames mutagenesis | - | 0.83 | - | 0.74 | - | 0.82 |
| Human Ether-a-go-go-Related Gene inhibition | + | 0.6847 | + | 0.6904 | + | 0.7077 |
| Micronuclear | + | 0.89 | + | 0.72 | + | 0.85 |
| Hepatotoxicity | + | 0.658 | - | 0.5331 | + | 0.7016 |
| skin sensitisation | - | 0.9032 | - | 0.8749 | - | 0.8965 |
| Respiratory toxicity | + | 0.7889 | + | 0.8889 | + | 0.8333 |
| Reproductive toxicity | + | 0.9778 | + | 0.8778 | + | 0.9778 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Mitochondrial toxicity | + | 0.8375 | + | 0.9375 | + | 0.8625 |
| Nephrotoxicity | - | 0.7813 | - | 0.8487 | - | 0.8256 |
| Acute Oral Toxicity (c) | III | 0.5346 | III | 0.6196 | III | 0.4304 |
| Estrogen receptor binding | + | 0.8058 | - | 0.5068 | + | 0.6955 |
| Androgen receptor binding | + | 0.7562 | + | 0.7281 | + | 0.7535 |
| Thyroid receptor binding | + | 0.552 | + | 0.7372 | + | 0.623 |
| Glucocorticoid receptor binding | - | 0.4766 | + | 0.809 | + | 0.7076 |
| Aromatase binding | + | 0.6353 | + | 0.7918 | + | 0.7016 |
| PPAR gamma | + | 0.7302 | + | 0.7904 | + | 0.7254 |
| □ | □ | □ | □ | □ | □ | □ |
| ADMET predicted profile-- Regressions | Value | Unit | Value | Unit | Value | Unit |
| Water solubility | -3.064 | logS | -2.295 | logS | -3.307 | logS |
| Plasma protein binding | 0.494 | 100% | 0.478 | 100% | 0.642 | 100% |
| Acute Oral Toxicity | 2.773 | log(1/(mol/kg)) | 3.294 | log(1/(mol/kg)) | 2.96 | log(1/(mol/kg)) |

Supplementary table. 3 List of 371 metabolites in the brain tissues of mice

| name | ID | formula | Con_Mean | Q-Con_Mean | T3-50 mg/kg.BW.d$^{-1}$_Mean | P.value | -log10(p) | FDR | VIP | pos/neg |
|---|---|---|---|---|---|---|---|---|---|---|
| 2-Hydroxyglutarate | M147T80 | C5H8O5 | 113553811.820 | 79812045.130 | 43377424.000 | 0.001 | 2.900 | 0.635 | 3.101 | neg |
| 25-Hydroxycholesterol | M401T538 | C27H46O2 | 3973150.840 | 198455.740 | 246064.510 | 0.007 | 2.130 | 0.635 | 2.504 | neg |
| Oleamide | M282T695 | C18H35NO | 4784628.170 | 6260735.990 | 513551.910 | 0.003 | 2.490 | 0.940 | 2.467 | pos |
| 4,5-Dihydroorotic acid | M159T58 | C5H6N2O4 | 65543222.650 | 45486988.620 | 39207581.230 | 0.018 | 1.740 | 0.940 | 2.329 | pos |
| Carnosine | M227T82 | C9H14N4O3 | 54705737.940 | 14393850.620 | 15250073.540 | 0.009 | 2.060 | 0.940 | 2.306 | pos |
| Gluconic acid | M195T80 | C6H12O7 | 57696227.670 | 59715827.220 | 62160589.490 | 0.057 | 1.240 | 0.639 | 2.259 | neg |
| gamma-Aminobutyric acid | M104T85 | C4H9NO2 | 2874851059.560 | 5804251395.080 | 5850952382.190 | 0.050 | 1.300 | 0.940 | 2.169 | pos |
| Taurohyocholate | M498T603 | C26H45NO7S | 2565302.810 | 1824615.400 | 497121.030 | 0.038 | 1.420 | 0.940 | 2.158 | pos |
| Deoxyuridine | M228T737 | C9H12N2O5 | 800011157.990 | 506438345.420 | 361069360.580 | 0.096 | 1.020 | 0.940 | 2.146 | pos |
| L-Malic acid | M133T72 | C4H6O5 | 1827421809.760 | 799593942.990 | 586963787.050 | 0.085 | 1.070 | 0.654 | 2.068 | neg |
| Maleamate | M114T74 | C4H5NO3 | 327840414.490 | 474390677.100 | 763565715.720 | 0.036 | 1.440 | 0.635 | 2.054 | neg |
| L-Kynurenine | M209T322 | C10H12N2O3 | 23046629.470 | 18391353.600 | 10847345.210 | 0.075 | 1.130 | 0.940 | 2.020 | pos |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| L-Glutamine | M145T98 | C5H10N2O3 | 92071322.225 | 105114125.929 | 69139929.270 | 0.040 | 1.390 | 0.635 | 1.994 | neg |
| Isocitric acid | M192T114 | C6H8O7 | 69403978.300 | 60562635.630 | 38642637.210 | 0.042 | 1.380 | 0.940 | 1.986 | pos |
| L-Lysine | M147T101 | C6H14N2O2 | 1483960362.620 | 1466135813.770 | 745984613.540 | 0.047 | 1.330 | 0.940 | 1.981 | pos |
| Xanthosine | M283T126_2 | C10H12N4O6 | 9073121.780 | 8669364.890 | 3833127.610 | 0.038 | 1.420 | 0.635 | 1.981 | neg |
| N-Acetyl-L-aspartic acid | M176T118 | C6H9NO5 | 1696037784.900 | 1659872101.510 | 1156992734.500 | 0.182 | 0.740 | 0.940 | 1.900 | pos |
| Guanosine | M284T264 | C10H13N5O5 | 1065332224.270 | 990139617.950 | 713292729.820 | 0.250 | 0.600 | 0.940 | 1.874 | pos |
| Butyryl-L-carnitine | M232T366 | C11H21NO4 | 34890205.890 | 35609552.010 | 29650525.100 | 0.385 | 0.410 | 0.940 | 1.832 | pos |
| gamma-Glutamylalanine | M219T135 | C7H11N2O5R | 15123450.270 | 49381715.220 | 53165910.290 | 0.029 | 1.530 | 0.940 | 1.810 | pos |
| Alpha-D-Glucose | M179T301 | C6H12O6 | 17814994.820 | 11225646.120 | 8151070.080 | 0.095 | 1.020 | 0.654 | 1.788 | neg |
| Beta-Leucine | M132T494 | C6H13NO2 | 9627679.950 | 8596438.910 | 7966370.380 | 0.090 | 1.050 | 0.940 | 1.770 | pos |
| Erucic acid | M338T810 | C22H42O2 | 6309367.620 | 5917328.020 | 3969308.520 | 0.103 | 0.990 | 0.940 | 1.768 | pos |
| Pyridoxamine | M169T331 | C8H12N2O2 | 63306953.370 | 60203034.550 | 37308205.380 | 0.236 | 0.630 | 0.940 | 1.754 | pos |
| S-Lactoylglutathione | M380T235 | C13H21N3O8S | 34850169.260 | 23344718.140 | 18832442.000 | 0.160 | 0.790 | 0.940 | 1.725 | pos |
| D-Arabitol | M133T506 | C5H12O5 | 17166383.730 | 16942388.190 | 15057534.790 | 0.078 | 1.110 | 0.651 | 1.704 | neg |
| (R)-4-Hydroxymandelate | M169T134 | C8H8O4 | 31222712.700 | 57841120.750 | 9280118.230 | 0.019 | 1.720 | 0.940 | 1.679 | pos |
| Mandelic acid | M151T596 | C8H8O3 | 4001907.650 | 4133363.330 | 2728283.660 | 0.144 | 0.840 | 0.702 | 1.635 | neg |
| Succinic acid | M117T74 | C4H6O4 | 314773005.010 | 257039402.390 | 195802833.910 | 0.203 | 0.690 | 0.726 | 1.631 | neg |

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|---|---|---|---|---|---|---|---|---|---|---|
| Dopamine | M136T179 | C8H11NO2 | 100982381.540 | 97533057.800 | 69595031.060 | 0.054 | 1.270 | 0.940 | 1.629 | pos |
| Hydroquinone | M110T733 | C6H6O2 | 46798971.290 | 42826676.310 | 34251747.820 | 0.149 | 0.830 | 0.940 | 1.624 | pos |
| Genistein | M270T431 | C15H10O5 | 9157516.620 | 6643769.520 | 6587248.430 | 0.172 | 0.760 | 0.704 | 1.619 | neg |
| N7-Methylguanosine | M298T325 | C11H16N5O5 | 14282309.840 | 13250958.330 | 6464029.440 | 0.117 | 0.930 | 0.940 | 1.610 | pos |
| | | C27H33N9O15 | | | | | | | | |
| FAD | M786T391_2 | P2 | 34302578.680 | 37055126.190 | 15004239.410 | 0.014 | 1.840 | 0.940 | 1.606 | pos |
| L-Phenylalanine | M166T328 | C9H11NO2 | 9181777035.710 | 6017910289.850 | 5532645854.810 | 0.114 | 0.940 | 0.940 | 1.602 | pos |
| 4a-Carbinolamine | | | | | | | | | | |
| tetrahydrobiopterin | M239T257 | C9H13N5O3 | 19184567.140 | 20429221.370 | 10961337.330 | 0.143 | 0.850 | 0.940 | 1.600 | pos |
| 4-Hydroxyphenyl-2- | | | | | | | | | | |
| propionic acid | M165T588 | C9H10O3 | 7755292.280 | 11645957.490 | 12902712.940 | 0.236 | 0.630 | 0.737 | 1.593 | neg |
| | | C14H26N4O11 | | | | | | | | |
| Citicoline | M489T87_1 | P2 | 28624368.490 | 20557587.030 | 23503424.560 | 0.291 | 0.540 | 0.940 | 1.586 | pos |
| 1-Methyladenosine | M282T325 | C11H15N5O4 | 50345396.630 | 30177905.650 | 23936584.590 | 0.587 | 0.230 | 0.940 | 1.578 | pos |
| N2-Succinyl-L-glutamic | | | | | | | | | | |
| acid 5-semialdehyde | M231T112 | C9H13NO6 | 21833025.530 | 21477145.590 | 14746063.850 | 0.402 | 0.400 | 0.940 | 1.570 | pos |
| Methylmalonic acid | M117T476 | C4H6O4 | 44311756.590 | 35182018.620 | 19288393.480 | 0.077 | 1.110 | 0.651 | 1.568 | neg |

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|---|---|---|---|---|---|---|---|---|---|---|
| 5-Keto-D-gluconate | M193T233 | C6H10O7 | 1071015.080 | 1018793.000 | 778085.820 | 0.229 | 0.640 | 0.737 | 1.559 | neg |
| Indoleacetaldehyde | M160T302 | C10H9NO | 53359897.690 | 31833220.220 | 25681792.160 | 0.104 | 0.980 | 0.940 | 1.548 | pos |
| L-Valine | M118T61 | C5H11NO2 | 32116246.020 | 39594034.150 | 23056111.380 | 0.069 | 1.160 | 0.940 | 1.544 | pos |
| gamma-Glutamyl-beta-aminopropiononitrile | M200T317 | C8H13N3O3 | 19452852.300 | 18739525.310 | 15345995.720 | 0.250 | 0.600 | 0.940 | 1.542 | pos |
| Glutathione | M307T211 | C10H17N3O6S | 347608235.030 | 358012225.440 | 171454994.940 | 0.144 | 0.840 | 0.940 | 1.540 | pos |
| Corticosterone | M347T704_1 | C21H30O4 | 20672162.370 | 28169530.820 | 10464926.130 | 0.095 | 1.020 | 0.940 | 1.539 | pos |
| 4-Hydroxybenzoic acid | M137T569 | C7H6O3 | 6435141.950 | 8721374.710 | 10228917.550 | 0.372 | 0.430 | 0.778 | 1.533 | neg |
| Oxybutynin | M358T738 | C22H31NO3 | 10791599.550 | 9099544.660 | 4612307.050 | 0.278 | 0.560 | 0.940 | 1.518 | pos |
| N-methyl-L-glutamic Acid | M162T115 | C6H11NO4 | 319988465.410 | 353957564.560 | 207883841.120 | 0.051 | 1.290 | 0.940 | 1.518 | pos |
| Glycocholic acid | M466T820 | C26H43NO6 | 27153606.850 | 24068284.110 | 15998905.490 | 0.291 | 0.540 | 0.940 | 1.517 | pos |
| Fisetin | M286T745 | C15H10O6 | 114937328.840 | 127444781.630 | 82860004.990 | 0.504 | 0.300 | 0.940 | 1.508 | pos |
| L-Glutamic gamma-semialdehyde | M131T150 | C5H9NO3 | 50834074.890 | 54128373.170 | 36739428.520 | 0.220 | 0.660 | 0.940 | 1.496 | pos |
| Uracil | M113T121 | C4H4N2O2 | 359045497.270 | 310345960.960 | 217025080.480 | 0.075 | 1.130 | 0.940 | 1.481 | pos |
| Pyroglutamic acid | M128T284 | C5H7NO3 | 12356507.230 | 91301631.010 | 74788164.690 | 0.024 | 1.620 | 0.635 | 1.475 | neg |
| N- | M434T287 | C16H23N3O11 | 11466160.960 | 22761578.280 | 18289809.170 | 0.281 | 0.550 | 0.940 | 1.475 | pos |

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|---|---|---|---|---|---|---|---|---|---|---|
| Acetylaspartylglutamylglut amate | | | | | | | | | | |
| (R)-Pantolactone | M132T822 | C6H10O3 | 3947151.850 | 4250819.660 | 3069575.630 | 0.042 | 1.370 | 0.940 | 1.474 | pos |
| | | C10H15N5O11 | | | | | | | | |
| GDP | M444T125_2 | P2 | 33693307.870 | 25678779.060 | 19691583.030 | 0.312 | 0.510 | 0.940 | 1.452 | pos |
| Uridine | M245T167 | C9H12N2O6 | 111322846.050 | 121455961.910 | 76194926.720 | 0.172 | 0.760 | 0.940 | 1.438 | pos |
| Riboflavin | M377T444_1 | C17H20N4O6 | 25613337.310 | 25974967.540 | 11992385.010 | 0.062 | 1.210 | 0.940 | 1.433 | pos |
| L-Glutamic acid | M148T85 | C5H9NO4 | 5632756439.320 | 1622348075.100 | 2647620021.770 | 0.119 | 0.920 | 0.940 | 1.427 | pos |
| gamma-L-Glutamyl-D- alanine | M218T369 | C8H14N2O5 | 16053895.860 | 15626465.040 | 12212351.480 | 0.470 | 0.330 | 0.940 | 1.425 | pos |
| 5,6-Dihydro-5-fluorouracil | M133T118 | C4H5FN2O2 | 239585508.630 | 257225307.260 | 188692423.660 | 0.075 | 1.130 | 0.940 | 1.421 | pos |
| 4-Hydroxybutanoic acid | M104T141 | C4H8O3 | 17887281.000 | 17963802.870 | 14365216.930 | 0.805 | 0.090 | 0.954 | 1.410 | pos |
| 7,8-Dihydromonapterin | M256T111 | C9H13N5O4 | 26020237.640 | 24838747.210 | 13475705.340 | 0.423 | 0.370 | 0.940 | 1.409 | pos |
| 8-Amino-7-oxononanoate | M170T482 | C9H17NO3 | 13512811.560 | 14165638.450 | 9906532.200 | 0.114 | 0.940 | 0.940 | 1.400 | pos |
| Beta-Tyrosine | M182T394 | C9H11NO3 | 25281943.760 | 22974793.600 | 19069369.100 | 0.587 | 0.230 | 0.940 | 1.393 | pos |
| Gulonic acid | M195T358 | C6H12O7 | 2128852.700 | 3011151.150 | 3305857.650 | 0.181 | 0.740 | 0.719 | 1.389 | neg |
| Triethylamine | M101T113 | C6H15N | 16477672.470 | 12517968.260 | 9899618.650 | 0.372 | 0.430 | 0.940 | 1.388 | pos |

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|---|---|---|---|---|---|---|---|---|---|---|
| N-Acetylleucine | M174T657 | C8H15NO3 | 13717706.710 | 8996180.070 | 9695083.070 | 0.244 | 0.610 | 0.940 | 1.387 | pos |
| alpha-Tocopherol | M430T523_2 | C29H50O2 | 40410353.250 | 37267942.800 | 27185819.450 | 0.653 | 0.190 | 0.943 | 1.383 | pos |
| 8,9-EET | M319T828 | C20H32O3 | 80711037.790 | 41265864.630 | 85034019.600 | 0.051 | 1.290 | 0.635 | 1.383 | neg |
| 9,10-Epoxyoctadecenoic acid | M295T824 | C18H32O3 | 36971030.470 | 36402496.070 | 30932069.680 | 0.623 | 0.210 | 0.861 | 1.382 | neg |
| 4-Pyridoxic acid | M182T333 | C8H9NO4 | 73246205.070 | 47161584.820 | 50084802.540 | 0.173 | 0.760 | 0.704 | 1.380 | neg |
| Ribose 1,5-bisphosphate | M309T785 | C5H12O11P2 | 4788347.200 | 4896270.290 | 3498075.750 | 0.203 | 0.690 | 0.726 | 1.370 | neg |
| Adenine | M136T126 | C5H5N5 | 34012381.280 | 42901271.720 | 10712572.950 | 0.039 | 1.410 | 0.940 | 1.365 | pos |
| 3-Hydroxymethylglutaric acid | M145T819 | C6H10O5 | 16227746.440 | 11622535.060 | 25237993.720 | 0.064 | 1.190 | 0.940 | 1.364 | pos |
| Cytidine | M243T296 | C9H13N3O5 | 47391023.880 | 49024788.290 | 35078000.690 | 0.109 | 0.960 | 0.940 | 1.361 | pos |
| Uric acid | M167T102 | C5H4N4O3 | 23247266.060 | 14642844.720 | 16191645.340 | 0.109 | 0.960 | 0.681 | 1.358 | neg |
| AICAR | M339T112 | C9H15N4O8P | 7935843.950 | 8438355.250 | 5176047.150 | 0.323 | 0.490 | 0.940 | 1.355 | pos |
| (S)-4-Hydroxymandelate | M151T69_2 | C8H8O4 | 1584478491.370 | 1504979181.990 | 1245350540.840 | 0.700 | 0.150 | 0.947 | 1.341 | pos |
| D-Erythrose 4-phosphate | M199T65 | C4H9O7P | 6559220.790 | 7127821.280 | 5326454.140 | 0.065 | 1.190 | 0.639 | 1.341 | neg |
| Dethiobiotin | M215T230 | C10H18N2O3 | 29037733.920 | 32084334.460 | 18434239.930 | 0.444 | 0.350 | 0.940 | 1.338 | pos |
| Acetylcysteine | M163T33 | C5H9NO3S | 24867562.740 | 23870364.420 | 30935148.870 | 0.042 | 1.380 | 0.940 | 1.333 | pos |

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|---|---|---|---|---|---|---|---|---|---|---|
| Erythritol | M121T485 | C4H10O4 | 15573145.560 | 19867584.920 | 7227223.100 | 0.062 | 1.210 | 0.639 | 1.328 | neg |
| (6Z)-Octadecenoic acid | M281T838 | C18H34O2 | 27324163.480 | 18931197.360 | 18181931.620 | 0.372 | 0.430 | 0.778 | 1.323 | neg |
| N-Acetyl-D-galactosamine | M204T96 | C8H15NO6 | 23950235.040 | 26055845.870 | 28206369.120 | 0.519 | 0.280 | 0.940 | 1.314 | pos |
| L-Asparagine | M133T100 | C4H8N2O3 | 27762593.540 | 24649428.980 | 21242532.300 | 0.623 | 0.210 | 0.943 | 1.312 | pos |
| 5-KETE | M319T691 | C20H30O3 | 4923682.490 | 5472285.150 | 5969230.560 | 0.738 | 0.130 | 0.948 | 1.301 | pos |
| 1-Hydroxymethylnaphthalene | M141T99 | C11H10O | 19335771.510 | 15231862.720 | 29492231.020 | 0.121 | 0.920 | 0.940 | 1.299 | pos |
| D-synephrine | M168T328 | C9H13NO2 | 25679700.070 | 26759119.510 | 21030240.930 | 0.751 | 0.120 | 0.948 | 1.272 | pos |
| 2-Hydroxybutyric acid | M104T118 | C4H8O3 | 106174063.380 | 92803491.530 | 79856998.870 | 0.459 | 0.340 | 0.940 | 1.262 | pos |
| Nicotianamine | M304T155 | C12H21N3O6 | 13634297.730 | 12815942.750 | 7934565.130 | 0.359 | 0.440 | 0.940 | 1.258 | pos |
| Phosphonoacetate | M140T59_2 | C2H5O5P | 214517230.860 | 156836625.440 | 268787271.090 | 0.067 | 1.180 | 0.940 | 1.250 | pos |
| Glycyl-leucine | M189T354 | C8H16N2O3 | 49409756.300 | 53413898.930 | 39589953.550 | 0.641 | 0.190 | 0.943 | 1.250 | pos |
| 2,3-Butanediol | M155T734 | C4H10O2S2 | 7174845.380 | 6215310.940 | 5227571.950 | 0.548 | 0.260 | 0.940 | 1.248 | pos |
| L-Arginine | M175T82 | C6H14N4O2 | 761741561.100 | 781928277.290 | 724475560.000 | 0.459 | 0.340 | 0.940 | 1.245 | pos |
| N6-(L-1,3-Dicarboxypropyl)-L-lysine | M277T83 | C11H20N2O6 | 14165072.340 | 14118225.500 | 15421929.340 | 0.372 | 0.430 | 0.940 | 1.237 | pos |
| S-Adenosylhomocysteine | M383T305_1 | C14H20N6O5S | 26641969.910 | 28473954.820 | 10958885.360 | 0.104 | 0.980 | 0.672 | 1.236 | neg |

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|---|---|---|---|---|---|---|---|---|---|---|
| D-Fructose | M179T220 | C6H12O6 | 14430184.110 | 15380691.420 | 11692947.460 | 0.203 | 0.690 | 0.726 | 1.230 | neg |
| Glucaric acid | M191T232 | C6H10O8 | 1396575.140 | 2617889.500 | 2777042.400 | 0.347 | 0.460 | 0.778 | 1.216 | neg |
| Deoxycorticosterone acetate | M371T798 | C23H32O4 | 1990769.190 | 3641366.050 | 1662536.380 | 0.423 | 0.370 | 0.795 | 1.216 | neg |
| Serotonin | M177T302 | C10H12N2O | 9708584.320 | 10094307.170 | 5880295.910 | 0.421 | 0.380 | 0.940 | 1.216 | pos |
| Maslinic acid | M472T790_2 | C30H48O4 | 4066529.110 | 6530102.940 | 5331896.750 | 0.209 | 0.680 | 0.940 | 1.216 | pos |
| Citrinin | M249T564 | C13H14O5 | 1304169.350 | 1228292.550 | 998000.630 | 0.738 | 0.130 | 0.895 | 1.214 | neg |
| Oxalureate | M133T133 | C3H4N2O4 | 79999661.200 | 74448456.310 | 64916555.990 | 0.519 | 0.280 | 0.940 | 1.213 | pos |
| 6-Hydroxynicotinic acid | M138T596 | C6H5NO3 | 10020472.180 | 9502265.090 | 8530852.680 | 0.347 | 0.460 | 0.778 | 1.212 | neg |
| 2-Aminophenol | M110T59 | C6H7NO | 17882203.840 | 16893010.530 | 14490148.680 | 0.281 | 0.550 | 0.940 | 1.212 | pos |
| Aminohydroquinone | M126T59 | C6H7NO2 | 30487123.830 | 30138584.030 | 48265064.690 | 0.414 | 0.380 | 0.940 | 1.211 | pos |
| Dehypoxanthine futalosine | M296T84 | C14H16O7 | 85265724.700 | 162316828.630 | 65277662.580 | 0.548 | 0.260 | 0.940 | 1.211 | pos |
| gamma-Amino-gamma-cyanobutanoate | M129T107 | C5H8N2O2 | 31141797.160 | 28695262.870 | 24366600.800 | 0.612 | 0.210 | 0.943 | 1.208 | pos |
| Oleic acid | M282T805 | C18H34O2 | 205992629.850 | 151902050.440 | 120425028.080 | 0.172 | 0.760 | 0.940 | 1.208 | pos |
| 10-Hydroxydecanoic acid | M187T579 | C10H20O3 | 5511591.660 | 5090970.770 | 4713301.090 | 0.312 | 0.510 | 0.772 | 1.204 | neg |
| Oxalacetic acid | M113T89 | C4H4O5 | 460980202.990 | 668957667.840 | 613092429.400 | 0.164 | 0.780 | 0.704 | 1.203 | neg |
| Porphobilinogen | M226T683 | C10H14N2O4 | 11195162.220 | 20003238.450 | 20017847.890 | 0.172 | 0.760 | 0.940 | 1.195 | pos |

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|---|---|---|---|---|---|---|---|---|---|---|
| Taurocholic acid | M498T661 | C26H45NO7S | 4264177.210 | 4617768.940 | 2487133.480 | 0.250 | 0.600 | 0.940 | 1.194 | pos |
| ADP | M428T100_2 | C10H15N5O10P2 | 104313575.450 | 120973530.290 | 73233306.520 | 0.529 | 0.280 | 0.940 | 1.186 | pos |
| 5-Hydroxy-L-tryptophan | M220T118 | C11H12N2O3 | 37499366.700 | 35547029.290 | 26470158.430 | 0.368 | 0.430 | 0.940 | 1.176 | pos |
| Lamivudine | M228T227 | C8H11N3O3S | 158286010.230 | 105805334.210 | 114897691.080 | 0.385 | 0.410 | 0.793 | 1.170 | neg |
| L-Tyrosine | M182T179 | C9H11NO3 | 1105980032.250 | 1124419352.650 | 1187617992.020 | 0.366 | 0.440 | 0.940 | 1.167 | pos |
| (-)-Epigallocatechin | M307T193 | C15H14O7 | 113060631.470 | 89560646.040 | 78819256.270 | 0.484 | 0.310 | 0.940 | 1.166 | pos |
| Phenyl acetate | M135T706 | C8H8O2 | 194517123.540 | 197944948.480 | 133136967.350 | 0.385 | 0.410 | 0.793 | 1.159 | neg |
| Hydroxykynurenine | M224T34 | C10H12N2O4 | 7271196.900 | 7601546.230 | 6507733.780 | 0.164 | 0.780 | 0.940 | 1.146 | pos |
| 1-Hexadecanol | M243T371 | C16H34O | 87043495.190 | 88000700.410 | 82851998.930 | 0.504 | 0.300 | 0.940 | 1.144 | pos |
| trans-Cinnamate | M147T317 | C9H8O2 | 8272752.500 | 9255215.310 | 5862560.140 | 0.130 | 0.890 | 0.702 | 1.142 | neg |
| N5-(L-1-Carboxyethyl)-L-ornithine | M204T506 | C8H16N2O4 | 24125158.760 | 25854385.130 | 15372138.730 | 0.641 | 0.190 | 0.943 | 1.138 | pos |
| Glyceric acid | M105T81 | C3H6O4 | 22649964.430 | 25316398.690 | 17069453.330 | 0.700 | 0.150 | 0.877 | 1.133 | neg |
| L-Serine | M104T83 | C3H7NO3 | 75878207.110 | 57230098.240 | 63089585.670 | 0.071 | 1.150 | 0.651 | 1.130 | neg |
| D-Xylitol | M133T525 | C5H12O5 | 19594046.620 | 20707250.110 | 16563133.770 | 0.318 | 0.500 | 0.772 | 1.128 | neg |
| Glutarate semialdehyde | M116T83 | C5H8O3 | 54271971.560 | 55666734.880 | 46673152.910 | 0.751 | 0.120 | 0.948 | 1.127 | pos |

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|---|---|---|---|---|---|---|---|---|---|---|
| Ribose 1-phosphate | M229T76 | C5H11O8P | 762976408.120 | 596302894.250 | 1002895641.500 | 0.060 | 1.220 | 0.639 | 1.123 | neg |
| Sorbitol | M183T33 | C6H14O6 | 18062776.820 | 14897776.170 | 14395007.880 | 0.459 | 0.340 | 0.940 | 1.122 | pos |
| N-Acetylaspartylglutamic acid | M305T231 | C11H16N2O8 | 32413579.410 | 35930859.980 | 23605260.340 | 0.366 | 0.440 | 0.940 | 1.122 | pos |
| Guanine | M152T146 | C5H5N5O | 111662686.720 | 83182107.780 | 78907934.280 | 0.368 | 0.430 | 0.940 | 1.120 | pos |
| 3-Hydroxybenzoate | M137T730 | C7H6O3 | 6606449.500 | 3334886.400 | 3472555.590 | 0.548 | 0.260 | 0.834 | 1.120 | neg |
| S-Carboxymethyl-L-cysteine | M162T300 | C5H9NO4S | 8371996.800 | 11649662.030 | 12417364.230 | 0.158 | 0.800 | 0.940 | 1.119 | pos |
| 5-Phosphoribosylamine | M228T410 | C5H12NO7P | 935748.550 | 1081457.870 | 559162.800 | 0.296 | 0.530 | 0.767 | 1.110 | neg |
| L-Carnitine | M162T102 | C7H15NO3 | 565425108.760 | 550729409.830 | 505393728.060 | 0.548 | 0.260 | 0.940 | 1.109 | pos |
| Nicotinamide ribotide | M334T722 | C11H15N2O8P | 13093840.720 | 11505602.970 | 15198169.100 | 0.135 | 0.870 | 0.940 | 1.105 | pos |
| Ribitol | M151T90 | C5H12O5 | 7459312.520 | 8671884.400 | 8821698.360 | 0.309 | 0.510 | 0.772 | 1.101 | neg |
| p-Aminobenzoic acid | M138T92 | C7H7NO2 | 20947718.100 | 22088304.960 | 15874260.210 | 0.281 | 0.550 | 0.940 | 1.096 | pos |
| 4-Methylaminobutyrate | M116T163 | C5H11NO2 | 1892488.390 | 1929005.510 | 1493404.140 | 0.459 | 0.340 | 0.814 | 1.093 | neg |
| 3-Carbamoyl-2-phenylpropionaldehyde | M193T162 | C10H11NO3 | 61287079.310 | 60382856.730 | 46673253.510 | 0.459 | 0.340 | 0.940 | 1.090 | pos |
| 4-Guanidinobutanoic acid | M146T247 | C5H11N3O2 | 8820068.500 | 45864878.500 | 22471687.810 | 0.169 | 0.770 | 0.940 | 1.084 | pos |

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|---|---|---|---|---|---|---|---|---|---|---|
| L-Aspartic acid | M134T132 | C4H7NO4 | 1474055367.390 | 1402248205.440 | 936588489.210 | 0.470 | 0.330 | 0.940 | 1.081 | pos |
| L-Tryptophan | M205T389 | C11H12N2O2 | 1528590187.020 | 1721531811.260 | 995798121.790 | 0.581 | 0.240 | 0.940 | 1.080 | pos |
| D-Tagaturonate | M193T132 | C6H10O7 | 1908919.650 | 1706926.510 | 1502937.730 | 0.079 | 1.100 | 0.651 | 1.077 | neg |
| N5-Methyl-L-glutamine | M161T94 | C6H12N2O3 | 13554196.450 | 13295398.550 | 12205916.790 | 0.587 | 0.230 | 0.940 | 1.076 | pos |
| 3-Methylindole | M132T170 | C9H9N | 61114902.040 | 41155586.520 | 43048541.160 | 0.366 | 0.440 | 0.940 | 1.076 | pos |
| 2-Hydroxy-2-ethylsuccinic acid | M161T589 | C6H10O5 | 30572715.300 | 12484071.240 | 14948998.380 | 0.262 | 0.580 | 0.751 | 1.062 | neg |
| Prostaglandin F2a | M353T594_1 | C20H34O5 | 67247958.120 | 89898878.130 | 142379756.910 | 0.431 | 0.370 | 0.802 | 1.061 | neg |
| (5-L-Glutamyl)-L-glutamate | M277T131 | C10H16N2O7 | 145962289.070 | 132427420.680 | 77052154.090 | 0.581 | 0.240 | 0.940 | 1.050 | pos |
| D-Galacturonate | M193T657 | C6H10O7 | 1019262.810 | 1165209.430 | 713055.690 | 0.318 | 0.500 | 0.772 | 1.040 | neg |
| Citric acid | M191T152 | C6H8O7 | 18820246.780 | 12489216.050 | 10672519.810 | 0.459 | 0.340 | 0.814 | 1.039 | neg |
| Undecanoic acid | M187T57 | C11H22O2 | 42358506.880 | 33549527.760 | 32736069.830 | 0.623 | 0.210 | 0.943 | 1.038 | pos |
| 3'-AMP | M346T283 | C10H14N5O7P | 2018297.820 | 2186108.770 | 1523648.180 | 0.385 | 0.410 | 0.793 | 1.028 | neg |
| gamma-L-Glutamyl-L-cysteinyl-beta-alanine | M322T179 | C11H19N3O6S | 97831276.340 | 84452034.950 | 60062412.580 | 0.645 | 0.190 | 0.943 | 1.021 | pos |
| L-3-Phenyllactic acid | M165T785 | C9H10O3 | 6629494.320 | 4191681.280 | 4337381.760 | 0.421 | 0.380 | 0.795 | 1.005 | neg |

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|---|---|---|---|---|---|---|---|---|---|---|
| L-Erythrulose | M119T100 | C4H8O4 | 19565059.230 | 14617207.580 | 15092491.790 | 0.587 | 0.230 | 0.834 | 1.004 | neg |
| Pantothenol | M206T349 | C9H19NO4 | 7075355.160 | 6000216.330 | 6231341.650 | 0.567 | 0.250 | 0.940 | 1.003 | pos |
| L-Histidine | M156T82_2 | C6H9N3O2 | 178572604.200 | 190644503.740 | 151316868.320 | 0.884 | 0.050 | 0.966 | 1.002 | pos |
| L-Methionine | M148T145 | C5H11NO2S | 5709173.590 | 5612596.950 | 4295849.950 | 0.692 | 0.160 | 0.877 | 1.000 | neg |
| 1H-Indole-3-carboxaldehyde | M144T572 | C9H7NO | 9887802.750 | 10513571.620 | 11947165.780 | 0.347 | 0.460 | 0.778 | 0.998 | neg |
| Rosmarinic acid | M360T452 | C18H16O8 | 3600429.010 | 3608187.370 | 2338394.960 | 0.359 | 0.440 | 0.940 | 0.994 | pos |
| (R)-5,6-Dihydrothymine | M128T59 | C5H8N2O2 | 17040506.010 | 18204908.870 | 14532181.600 | 0.911 | 0.040 | 0.974 | 0.991 | pos |
| Niacinamide | M123T396 | C6H6N2O | 22916228.390 | 24399497.760 | 19793687.420 | 0.864 | 0.060 | 0.966 | 0.991 | pos |
| 2-Furoate | M111T67 | C5H4O3 | 161147735.500 | 144585422.640 | 136642437.460 | 0.927 | 0.030 | 0.965 | 0.989 | neg |
| Nitrendipine | M361T548_1 | C18H20N2O6 | 26844279.580 | 24269772.930 | 16743868.790 | 0.630 | 0.200 | 0.943 | 0.983 | pos |
| Uridine diphosphate glucuronic acid | M579T69_1 | C15H22N2O18P2 | 8588760.260 | 14068985.100 | 4583752.270 | 0.095 | 1.020 | 0.654 | 0.981 | neg |
| 1-Aminocyclopropanecarboxylic acid | M102T104 | C4H7NO2 | 119152265.380 | 175643378.630 | 88889546.870 | 0.312 | 0.510 | 0.940 | 0.978 | pos |
| 19(S)-HETE | M319T803 | C20H32O3 | 6383554.650 | 4556012.350 | 5984575.000 | 0.444 | 0.350 | 0.812 | 0.965 | neg |

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|---|---|---|---|---|---|---|---|---|---|---|
| 9,10-DHOME | M313T752 | C18H34O4 | 13973181.340 | 11082200.890 | 11969939.910 | 0.796 | 0.100 | 0.916 | 0.964 | neg |
| D-Myo-inositol 4-phosphate | M259T73 | C6H13O9P | 291787013.850 | 401530734.700 | 192602336.890 | 0.130 | 0.890 | 0.702 | 0.961 | neg |
| Phosphorylcholine | M184T83 | C5H15NO4P | 1001873034.010 | 1077447722.270 | 897750499.700 | 0.567 | 0.250 | 0.940 | 0.956 | pos |
| Palmitoyl-L-carnitine | M400T796 | C23H45NO4 | 865962448.940 | 786378791.390 | 637430913.570 | 0.504 | 0.300 | 0.940 | 0.956 | pos |
| 3-Methoxytyramine | M168T304 | C9H13NO2 | 21635528.710 | 23186978.100 | 13902619.800 | 0.128 | 0.890 | 0.940 | 0.954 | pos |
| myo-Inositol | M179T96 | C6H12O6 | 32092882.820 | 32000054.830 | 29928194.170 | 0.676 | 0.170 | 0.877 | 0.950 | neg |
| Dehydroascorbate | M173T110 | C6H6O6 | 106795329.060 | 109894193.560 | 88941371.440 | 0.849 | 0.070 | 0.932 | 0.947 | neg |
| 3-Hydroxyanthranilate | M152T687 | C7H7NO3 | 4754440.440 | 4654812.480 | 3995298.840 | 0.717 | 0.140 | 0.884 | 0.947 | neg |
| DL-Glutamate | M128T246 | C5H9NO4 | 26329652.030 | 32454258.180 | 15120906.510 | 0.523 | 0.280 | 0.823 | 0.946 | neg |
| 2-Hydroxycinnamic acid | M165T121 | C9H8O3 | 270921109.350 | 219891617.470 | 203796938.750 | 0.805 | 0.090 | 0.954 | 0.945 | pos |
| Acetylcholine | M146T108 | C7H16NO2 | 279055323.120 | 299390498.830 | 243676070.290 | 0.927 | 0.030 | 0.974 | 0.937 | pos |
| N-Acetyl-D-glucosamine | M220T100 | C8H15NO6 | 14928119.820 | 15445810.050 | 12449300.880 | 0.692 | 0.160 | 0.877 | 0.922 | neg |
| N-Acetyl-L-glutamine | M188T439 | C7H12N2O4 | 1285178.250 | 289895.580 | 473628.770 | 0.459 | 0.340 | 0.814 | 0.920 | neg |
| N-Succinyl-L-citrulline | M276T94 | C10H17N3O6 | 130787752.090 | 78974110.210 | 65860563.110 | 0.700 | 0.150 | 0.947 | 0.919 | pos |
| Kanosamine | M162T133 | C6H13NO5 | 7064901.040 | 10205973.870 | 6737686.850 | 0.581 | 0.240 | 0.940 | 0.917 | pos |
| Threonic acid | M136T73 | C4H8O5 | 34148877.620 | 26509492.530 | 26570880.960 | 0.834 | 0.080 | 0.931 | 0.910 | neg |

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|---|---|---|---|---|---|---|---|---|---|---|
| Citramalic acid | M129T69 | C5H8O5 | 46316207.540 | 59013035.060 | 36482925.940 | 0.264 | 0.580 | 0.751 | 0.908 | neg |
| Arachidic acid | M311T773 | C20H40O2 | 9914459.680 | 25932934.020 | 18392882.840 | 0.236 | 0.630 | 0.737 | 0.907 | neg |
| 1H-Indole-3-acetamide | M173T147 | C10H10N2O | 11942353.090 | 22211903.410 | 8105157.400 | 0.359 | 0.440 | 0.778 | 0.905 | neg |
| L-Homophenylalanine | M180T645 | C10H13NO2 | 11224709.110 | 4460881.920 | 5341428.570 | 0.347 | 0.460 | 0.940 | 0.899 | pos |
| Kojic acid | M141T705 | C6H6O4 | 6033987.280 | 5557456.180 | 4968823.960 | 0.778 | 0.110 | 0.908 | 0.892 | neg |
| Phosphoenolpyruvic acid | M168T312 | C3H5O6P | 81048269.970 | 83526247.660 | 51246742.860 | 0.700 | 0.150 | 0.947 | 0.887 | pos |
| Phenylacetic acid | M135T392 | C8H8O2 | 20344237.080 | 20232585.080 | 18063738.240 | 0.612 | 0.210 | 0.857 | 0.882 | neg |
| Ethylmethylacetic acid | M101T719 | C5H10O2 | 22257479.800 | 19045260.720 | 16395863.560 | 0.581 | 0.240 | 0.834 | 0.882 | neg |
| Nonadecanoic acid | M297T837 | C19H38O2 | 33911698.210 | 33095834.440 | 30127947.730 | 0.645 | 0.190 | 0.861 | 0.880 | neg |
| Chavicol | M135T732 | C9H10O | 5230312.420 | 4502722.920 | 6667012.640 | 0.103 | 0.990 | 0.940 | 0.879 | pos |
| CMP | M322T80 | C9H14N3O8P | 19034681.660 | 34843076.880 | 8295015.590 | 0.082 | 1.080 | 0.651 | 0.875 | neg |
| Oxoadipic acid | M159T132 | C6H8O5 | 62181514.680 | 60434396.010 | 53253340.900 | 0.778 | 0.110 | 0.908 | 0.874 | neg |
| Linoleic acid | M279T746 | C18H32O2 | 10083266.010 | 10442882.050 | 5454949.150 | 0.067 | 1.180 | 0.650 | 0.869 | neg |
| N-Acetyl-L-phenylalanine | M206T375 | C11H13NO3 | 29595067.910 | 22073821.760 | 25363078.960 | 0.236 | 0.630 | 0.737 | 0.861 | neg |
| AMP | M348T135_1 | C10H14N5O7P | 260543328.190 | 180680458.770 | 160766790.630 | 0.612 | 0.210 | 0.943 | 0.848 | pos |
| Thiamine monophosphate | M344T73 | C12H18N4O4PS | 24783149.990 | 84227538.700 | 58617545.870 | 0.169 | 0.770 | 0.704 | 0.844 | neg |

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|---|---|---|---|---|---|---|---|---|---|---|
| Equol | M241T326 | C15H14O3 | 7824473.810 | 8744796.320 | 6653750.640 | 0.476 | 0.320 | 0.816 | 0.841 | neg |
| Sodium deoxycholate | M415T801 | C24H39O4. Na | 42903512.680 | 34157373.560 | 27392615.760 | 0.444 | 0.350 | 0.940 | 0.837 | pos |
| 3-Methyl-L-tyrosine | M195T821 | C10H13NO3 | 5593555.360 | 11700510.410 | 9379776.140 | 0.312 | 0.510 | 0.940 | 0.835 | pos |
| Cyclic AMP | M328T316 | C10H12N5O6P | 3600114.460 | 3825737.600 | 2549659.720 | 0.347 | 0.460 | 0.778 | 0.834 | neg |
| Citrulline | M176T105 | C6H13N3O3 | 70803447.270 | 102472119.440 | 94994709.060 | 0.630 | 0.200 | 0.943 | 0.827 | pos |
| N-Acetylglutamic acid | M188T77 | C7H11NO5 | 78697934.640 | 75356858.660 | 88619668.000 | 0.612 | 0.210 | 0.857 | 0.826 | neg |
| D-(+)-Glucose | M179T355 | C6H12O6 | 7112925.100 | 7140897.210 | 5269908.500 | 0.203 | 0.690 | 0.726 | 0.825 | neg |
| Anserine | M241T82 | C10H16N4O3 | 87154440.250 | 102738713.360 | 75041950.520 | 0.504 | 0.300 | 0.940 | 0.817 | pos |
| Stearic acid | M284T431 | C18H36O2 | 9459100.730 | 10540844.070 | 7830053.410 | 0.834 | 0.080 | 0.963 | 0.815 | pos |
| 11-Dehydrocorticosterone | M325T792 | C21H28O4 | 15411446.920 | 12010864.320 | 17777879.050 | 0.778 | 0.110 | 0.908 | 0.813 | neg |
| Pyrrolidonecarboxylic acid | M130T358 | C5H7NO3 | 10758355.930 | 12773226.110 | 7510792.720 | 0.312 | 0.510 | 0.940 | 0.804 | pos |
| Lichenin | M161T814 | C6H10O5 | 20399388.080 | 24549399.470 | 24872028.070 | 0.688 | 0.160 | 0.877 | 0.803 | neg |
| Aminocaproic acid | M130T701 | C6H13NO2 | 14320674.090 | 13527076.070 | 15846184.780 | 0.423 | 0.370 | 0.795 | 0.803 | neg |
| Ornithine | M133T73 | C5H12N2O2 | 11198633.510 | 14228916.700 | 9485081.750 | 0.148 | 0.830 | 0.940 | 0.802 | pos |
| Neocembrene | M273T742 | C20H32 | 27619283.650 | 29325392.800 | 31012012.220 | 0.810 | 0.090 | 0.954 | 0.799 | pos |
| 4-Oxoglutaramate | M145T433 | C5H7NO4 | 42150722.920 | 51754322.920 | 58529374.560 | 0.796 | 0.100 | 0.954 | 0.795 | pos |
| D-Galactose | M179T475 | C6H12O6 | 4616986.580 | 6532104.240 | 6744766.310 | 0.692 | 0.160 | 0.877 | 0.795 | neg |

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|---|---|---|---|---|---|---|---|---|---|---|
| Thymidine | M223T746 | C10H14N2O5 | 7054001.070 | 8655434.960 | 7548179.280 | 0.182 | 0.740 | 0.719 | 0.789 | neg |
| Indolelactic acid | M204T370_1 | C11H11NO3 | 3013645.730 | 2882228.520 | 2657611.300 | 0.810 | 0.090 | 0.916 | 0.786 | neg |
| 4-Hydroxycinnamic acid | M164T105_2 | C9H8O3 | 9441144.790 | 5174799.310 | 5237645.110 | 0.069 | 1.160 | 0.940 | 0.782 | pos |
| Pantothenic acid | M218T160 | C9H17NO5 | 250427482.720 | 289110835.480 | 204659643.650 | 0.493 | 0.310 | 0.823 | 0.779 | neg |
| Isonicotinic acid | M124T35 | C6H5NO2 | 17690285.190 | 19902068.690 | 15586774.560 | 0.140 | 0.850 | 0.940 | 0.779 | pos |
| 2-Methoxy-4-vinylphenol | M151T304 | C9H10O2 | 26724164.720 | 28320927.790 | 28089438.610 | 0.385 | 0.410 | 0.940 | 0.773 | pos |
| D-beta-Phenylalanine | M166T487 | C9H11NO2 | 5783192.100 | 5672466.860 | 4961073.140 | 0.895 | 0.050 | 0.966 | 0.772 | pos |
| Hypoxanthine | M135T129 | C5H4N4O | 598391926.410 | 735809993.760 | 783389779.670 | 0.641 | 0.190 | 0.861 | 0.772 | neg |
| D-Glucose | M179T464 | C6H12O6 | 2537054.170 | 2440800.630 | 2087976.590 | 0.751 | 0.120 | 0.895 | 0.770 | neg |
| 6-Keto-prostaglandin F1a | M369T522 | C20H34O6 | 29713245.000 | 20633934.870 | 30756567.010 | 0.523 | 0.280 | 0.823 | 0.764 | neg |
| 1,5-Naphthalenediamine | M159T389 | C10H10N2 | 26099320.850 | 31217498.690 | 23639031.260 | 0.529 | 0.280 | 0.940 | 0.761 | pos |
| Ergothioneine | M230T99 | C9H16N3O2S | 62155735.070 | 37964537.350 | 45570303.790 | 0.805 | 0.090 | 0.954 | 0.758 | pos |
| D-Mannuronate | M193T445 | C6H10O7 | 2277396.410 | 2034931.480 | 1486322.030 | 0.493 | 0.310 | 0.823 | 0.755 | neg |
| Ketoleucine | M129T322 | C6H10O3 | 7225358.130 | 12384163.250 | 9626311.020 | 0.318 | 0.500 | 0.772 | 0.752 | neg |
| Taurine | M126T103 | C2H7NO3S | 500335729.490 | 931457656.440 | 672213151.130 | 0.150 | 0.820 | 0.940 | 0.752 | pos |
| Cytidine monophosphate N-acetylneuraminic acid | M613T80_2 | C20H31N4O16P | 36030667.910 | 32824476.230 | 31139928.980 | 0.688 | 0.160 | 0.877 | 0.750 | neg |

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|---|---|---|---|---|---|---|---|---|---|---|
| Pyridoxine | M170T91 | C8H11NO3 | 515691104.370 | 483619812.480 | 544517251.890 | 0.834 | 0.080 | 0.963 | 0.734 | pos |
| Choline | M104T82 | C5H14NO | 3494094426.220 | 3223089428.510 | 3070977003.490 | 0.493 | 0.310 | 0.940 | 0.724 | pos |
| Ascorbate | M177T114 | C6H8O6 | 69023854.970 | 64441644.650 | 52951738.660 | 0.523 | 0.280 | 0.940 | 0.721 | pos |
| Allantoin | M157T94 | C4H6N4O3 | 7884694.740 | 6182327.820 | 6222781.500 | 0.359 | 0.440 | 0.778 | 0.716 | neg |
| trans-trans-Muconic acid | M125T59 | C6H6O4 | 25971600.550 | 29319453.810 | 19295376.830 | 0.343 | 0.460 | 0.940 | 0.712 | pos |
| L-Homocysteine | M135T270 | C4H9NO2S | 50610667.460 | 49980460.940 | 50225198.570 | 0.470 | 0.330 | 0.816 | 0.707 | neg |
| S-(Hydroxymethyl)glutathione | M337T139 | C11H19N3O7S | 3394825.350 | 4151867.570 | 3957173.380 | 0.548 | 0.260 | 0.940 | 0.700 | pos |
| 4'-Oxonebramine | M304T118_3 | C12H24N4O5 | 47791562.740 | 37793320.140 | 34370445.080 | 0.519 | 0.280 | 0.940 | 0.699 | pos |
| Phenylpropanoate | M149T609 | C9H10O2 | 1307172.680 | 3415505.650 | 1956196.930 | 0.091 | 1.040 | 0.654 | 0.698 | neg |
| 5-Hydroxyindoleacetic acid | M192T437 | C10H9NO3 | 17437830.160 | 15919655.230 | 14353251.260 | 0.805 | 0.090 | 0.954 | 0.697 | pos |
| 5'-Methylthioadenosine | M298T377_1 | C11H15N5O3S | 512148119.270 | 519529682.160 | 445308898.410 | 0.751 | 0.120 | 0.948 | 0.696 | pos |
| Dimethylglycine | M102T78 | C4H9NO2 | 22947506.030 | 37488430.730 | 26960721.150 | 0.128 | 0.890 | 0.702 | 0.694 | neg |
| Cyanuric acid | M129T167 | C3H3N3O3 | 44760978.740 | 36311537.940 | 40642782.570 | 0.587 | 0.230 | 0.834 | 0.686 | neg |
| Leucine | M132T239 | C6H13NO2 | 525745802.210 | 588611562.050 | 670430755.770 | 0.587 | 0.230 | 0.940 | 0.672 | pos |
| Inosine | M269T265 | C10H12N4O5 | 2336626736.680 | 3702407448.600 | 1458268553.180 | 0.135 | 0.870 | 0.940 | 0.657 | pos |

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|---|---|---|---|---|---|---|---|---|---|---|
| L-Threonine | M120T103 | C4H9NO3 | 115052558.060 | 103524049.110 | 70485347.750 | 0.717 | 0.140 | 0.948 | 0.656 | pos |
| Paxilline | M434T790 | C27H33NO4 | 2690886.330 | 6929709.550 | 3125925.890 | 0.008 | 2.090 | 0.635 | 0.647 | neg |
| Benzaldehyde | M107T328 | C7H6O | 12113153.980 | 14101683.120 | 13412010.940 | 0.778 | 0.110 | 0.954 | 0.641 | pos |
| Guanidinosuccinic acid | M175T184 | C5H9N3O4 | 26825050.810 | 20452397.570 | 26167728.820 | 0.281 | 0.550 | 0.751 | 0.632 | neg |
| Genistin | M432T801 | C21H20O10 | 14221876.870 | 22091433.370 | 13509511.060 | 0.864 | 0.060 | 0.966 | 0.627 | pos |
| L-Gulonolactone | M177T761 | C6H10O6 | 7004270.340 | 7545490.150 | 8086008.650 | 0.653 | 0.190 | 0.861 | 0.625 | neg |
| S-Glutathionyl-L-cysteine | M427T93 | C13H22N4O8S2 | 71949643.880 | 36072649.270 | 60196150.160 | 0.587 | 0.230 | 0.940 | 0.616 | pos |
| Amino acid(Arg-) | M173T151 | C6H14N4O2 | 32134684.640 | 35054950.320 | 30800273.670 | 0.229 | 0.640 | 0.737 | 0.594 | neg |
| Lumichrome | M243T561 | C12H10N4O2 | 27097506.050 | 35048999.540 | 21057835.920 | 0.224 | 0.650 | 0.940 | 0.593 | pos |
| 1-Methylhistamine | M126T71 | C6H11N3 | 32193474.540 | 32753786.210 | 36954880.030 | 0.676 | 0.170 | 0.947 | 0.587 | pos |
| Malonate | M103T90 | C3H4O4 | 15793525.660 | 15916208.210 | 15696286.690 | 0.229 | 0.640 | 0.737 | 0.583 | neg |
| (2R)-2-Hydroxy-3-(phosphonatooxy)propanoate | M185T69 | C3H7O7P | 82839583.060 | 51280998.080 | 74757795.080 | 0.065 | 1.190 | 0.639 | 0.578 | neg |
| Bufotenin | M204T310 | C12H16N2O | 11874033.850 | 13280104.280 | 11954767.780 | 0.994 | 0.000 | 0.995 | 0.566 | pos |
| Creatinine | M114T102 | C4H7N3O | 880262115.150 | 841341271.270 | 1203251769.540 | 0.805 | 0.090 | 0.954 | 0.560 | pos |

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|---|---|---|---|---|---|---|---|---|---|---|
| Salicylic acid | M137T641 | C7H6O3 | 9632282.320 | 11878723.510 | 8374004.570 | 0.884 | 0.050 | 0.948 | 0.557 | neg |
| Shikimic acid | M173T103 | C7H10O5 | 20154972.380 | 13778521.730 | 12845102.090 | 0.796 | 0.100 | 0.916 | 0.554 | neg |
| N-Formyl-L-methionine | M176T180 | C6H11NO3S | 3391891.050 | 3464839.840 | 4561595.370 | 0.630 | 0.200 | 0.861 | 0.551 | neg |
| | | C11H20N4O11 | | | | | | | | |
| CDP-Ethanolamine | M447T86 | P2 | 14306804.120 | 18010512.020 | 12281459.580 | 0.630 | 0.200 | 0.943 | 0.550 | pos |
| Aminoadipic acid | M160T79 | C6H11NO4 | 34575796.870 | 29957941.360 | 33199213.510 | 0.476 | 0.320 | 0.816 | 0.549 | neg |
| N-Acetyl-L-glutamate 5- | | | | | | | | | | |
| semialdehyde | M172T126 | C7H11NO4 | 7784215.640 | 4380624.780 | 6263756.150 | 0.587 | 0.230 | 0.834 | 0.548 | neg |
| Protoporphyrinogen IX | M568T834_2 | C34H40N4O4 | 137439143.520 | 250494238.200 | 203922679.210 | 0.581 | 0.240 | 0.940 | 0.548 | pos |
| N-Acetylornithine | M173T109 | C7H14N2O3 | 6880738.900 | 7198345.010 | 6672680.540 | 0.692 | 0.160 | 0.877 | 0.547 | neg |
| Beta-Glycerophosphoric | | | | | | | | | | |
| acid | M171T75 | C3H9O6P | 642127063.600 | 346192380.390 | 494568311.480 | 0.091 | 1.040 | 0.654 | 0.545 | neg |
| | | C14H18N5O11 | | | | | | | | |
| Adenylsuccinic acid | M464T301_1 | P | 52755946.270 | 55011650.540 | 23940419.310 | 0.220 | 0.660 | 0.940 | 0.534 | pos |
| Succinic acid semialdehyde | M101T786 | C4H6O3 | 8729527.460 | 9782358.420 | 7153438.500 | 0.523 | 0.280 | 0.823 | 0.533 | neg |
| 1-Pyrroline-2-carboxylic | | | | | | | | | | |
| acid | M114T513 | C5H7NO2 | 86438442.300 | 64000000.210 | 64807139.950 | 0.630 | 0.200 | 0.943 | 0.526 | pos |

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|---|---|---|---|---|---|---|---|---|---|---|
| Hydroxypyruvic acid | M103T80 | C3H4O4 | 32849720.100 | 30903137.180 | 39785331.050 | 0.688 | 0.160 | 0.877 | 0.519 | neg |
| L-Homoserine | M118T701 | C4H9NO3 | 2172452.730 | 2910452.630 | 2039555.860 | 0.250 | 0.600 | 0.743 | 0.514 | neg |
| 2,4-Dinitrophenol | M183T453 | C6H4N2O5 | 10030375.660 | 11567919.450 | 8576247.230 | 0.529 | 0.280 | 0.823 | 0.511 | neg |
| L-Altarate | M191T218 | C6H10O8 | 13326336.660 | 10103864.610 | 21238417.660 | 0.854 | 0.070 | 0.932 | 0.504 | neg |
| Deoxyinosine | M251T296 | C10H12N4O4 | 2335417.780 | 1915972.190 | 2293496.920 | 0.630 | 0.200 | 0.861 | 0.501 | neg |
| GMP | M364T136_1 | C10H14N5O8P | 69539707.150 | 113991746.860 | 43791454.780 | 0.113 | 0.950 | 0.940 | 0.500 | pos |
| (R)-3-Hydroxybutyric acid | M103T92 | C4H8O3 | 61389478.410 | 32367974.580 | 45010518.670 | 0.229 | 0.640 | 0.737 | 0.495 | neg |
| 4-Hydroxyphenylacetaldehyde | M136T90 | C8H8O2 | 58453281.240 | 66232830.670 | 55961027.910 | 0.717 | 0.140 | 0.948 | 0.491 | pos |
| 8-Hydroxyquinoline | M145T721 | C9H7NO | 69316857.710 | 69582865.830 | 83549764.540 | 0.895 | 0.050 | 0.966 | 0.475 | pos |
| Sphinganine | M302T754 | C18H39NO2 | 103728094.370 | 86024902.920 | 103396158.340 | 0.755 | 0.120 | 0.948 | 0.463 | pos |
| N-Alpha-acetyllysine | M188T389 | C8H16N2O3 | 1007575823.320 | 1317567818.970 | 956603756.010 | 0.630 | 0.200 | 0.943 | 0.459 | pos |
| N-Acetylhistidine | M198T169 | C8H11N3O3 | 21837596.110 | 21008183.790 | 19701246.900 | 0.700 | 0.150 | 0.947 | 0.454 | pos |
| Creatine | M130T97 | C4H9N3O2 | 967580102.710 | 830800656.630 | 855026723.230 | 0.612 | 0.210 | 0.857 | 0.451 | neg |
| Fructose 1,6-bisphosphate | M341T127 | C6H14O12P2 | 17298697.320 | 15215749.900 | 20798429.040 | 0.849 | 0.070 | 0.963 | 0.449 | pos |
| N2-Succinyl-L-ornithine | M232T434 | C9H16N2O5 | 12074991.960 | 13613778.380 | 13419389.970 | 0.983 | 0.010 | 0.991 | 0.446 | pos |

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|---|---|---|---|---|---|---|---|---|---|---|
| 3-(2-Hydroxyphenyl)propanoic acid | M165T618 | C9H10O3 | 5986601.340 | 5502241.200 | 6382343.360 | 0.700 | 0.150 | 0.877 | 0.444 | neg |
| Hippuric acid | M178T328 | C9H9NO3 | 25506351.510 | 23877344.320 | 24451550.960 | 0.849 | 0.070 | 0.932 | 0.441 | neg |
| Gentamicin C1a | M432T454 | C19H39N5O7 | 5684008.170 | 5756711.380 | 5545157.870 | 0.884 | 0.050 | 0.966 | 0.433 | pos |
| Xanthine | M151T160 | C5H4N4O2 | 451051003.140 | 486543286.240 | 439955859.090 | 0.158 | 0.800 | 0.704 | 0.431 | neg |
| Oxidized glutathione | M613T159_2 | C20H32N6O12S2 | 249828952.930 | 321147888.920 | 441360854.820 | 0.849 | 0.070 | 0.963 | 0.427 | pos |
| L-Norvaline | M116T113 | C5H11NO2 | 109331008.970 | 84525482.960 | 106950127.150 | 0.476 | 0.320 | 0.816 | 0.423 | neg |
| gamma-Glutamylcysteine | M249T88 | C8H14N2O5S | 26284371.670 | 19144525.410 | 24328880.930 | 0.343 | 0.460 | 0.778 | 0.418 | neg |
| FMN | M455T382_2 | C17H21N4O9P | 7683645.290 | 8670156.370 | 8037435.310 | 0.751 | 0.120 | 0.895 | 0.410 | neg |
| L-threo-3-Methylaspartate | M148T275 | C5H9NO4 | 22304584.550 | 37605378.790 | 18785368.430 | 0.109 | 0.960 | 0.940 | 0.404 | pos |
| Spermine | M203T73 | C10H26N4 | 11775742.730 | 9557682.410 | 11609170.970 | 0.755 | 0.120 | 0.948 | 0.401 | pos |
| Dehydroepiandrosterone | M288T737_2 | C19H28O2 | 7453870777.270 | 7099552702.120 | 10709134172.250 | 0.805 | 0.090 | 0.954 | 0.395 | pos |
| beta-Citryl-L-glutamate | M302T63 | C11H15NO10 | 39012774.040 | 57644278.080 | 46969831.120 | 0.630 | 0.200 | 0.861 | 0.385 | neg |
| Nopaline | M285T93 | C11H20N4O6 | 5418823.170 | 6476980.380 | 4653564.600 | 0.444 | 0.350 | 0.812 | 0.384 | neg |
| Oxoglutaric acid | M145T81 | C5H6O5 | 927726.750 | 2278278.830 | 1385786.890 | 0.090 | 1.050 | 0.654 | 0.378 | neg |

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|---|---|---|---|---|---|---|---|---|---|---|
| Glycitein | M283T146 | C16H12O5 | 1533044.580 | 2823110.330 | 1657168.510 | 0.250 | 0.600 | 0.743 | 0.363 | neg |
| Cortexolone | M346T756_1 | C21H30O4 | 57668386.300 | 48845085.720 | 72109481.510 | 0.385 | 0.410 | 0.940 | 0.360 | pos |
| Homocarnosine | M239T106 | C10H16N4O3 | 221768989.760 | 205308595.640 | 196558485.400 | 0.700 | 0.150 | 0.877 | 0.356 | neg |
| L-Gulose | M179T333 | C6H12O6 | 11871036.640 | 16009020.960 | 11922906.040 | 0.402 | 0.400 | 0.795 | 0.333 | neg |
| all-trans-Retinoic acid | M301T691 | C20H28O2 | 3795765.890 | 3482242.400 | 3743866.290 | 0.932 | 0.030 | 0.974 | 0.332 | pos |
| D-Phenylalanine | M164T301_2 | C9H11NO2 | 638962408.090 | 562090611.120 | 618870762.100 | 0.949 | 0.020 | 0.976 | 0.323 | neg |
| N6-Acetyl-L-lysine | M187T218 | C8H16N2O3 | 6858011.200 | 6190500.410 | 6930599.330 | 0.751 | 0.120 | 0.895 | 0.311 | neg |
| cis-4-Hydroxy-L-proline | M132T141 | C5H9NO3 | 612937155.480 | 782442495.020 | 402678369.730 | 0.077 | 1.110 | 0.940 | 0.308 | pos |
| Formononetin | M268T270 | C16H12O4 | 322730250.690 | 347605210.450 | 377679337.020 | 0.325 | 0.490 | 0.772 | 0.307 | neg |
| Glycerophosphocholine | M258T103 | C8H21NO6P | 237523605.930 | 255251537.520 | 212003694.270 | 0.688 | 0.160 | 0.947 | 0.306 | pos |
| 3,4-Methylenedioxyamphetamine | M194T303 | C11H15NO2 | 35699669.400 | 42517221.760 | 36593606.430 | 0.834 | 0.080 | 0.963 | 0.298 | pos |
| 4-Hydroxybenzaldehyde | M123T179 | C7H6O2 | 36709577.770 | 32030877.090 | 35557469.430 | 0.181 | 0.740 | 0.940 | 0.296 | pos |
| Acetylphosphate | M140T427 | C2H5O5P | 13416966.720 | 10686634.880 | 16576050.880 | 0.402 | 0.400 | 0.940 | 0.291 | pos |
| Thiazole | M279T425 | C11H8N2O3S2 | 4895079.870 | 6161231.470 | 4139714.000 | 0.366 | 0.440 | 0.778 | 0.286 | neg |
| Argininosuccinic acid | M291T84 | C10H18N4O6 | 8276789.210 | 24310978.170 | 16136409.310 | 0.312 | 0.510 | 0.940 | 0.275 | pos |

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|---|---|---|---|---|---|---|---|---|---|---|
| Anabasine | M145T808 | C10H14N2 | 14858762.430 | 8899726.680 | 14021493.930 | 0.278 | 0.560 | 0.940 | 0.273 | pos |
| Gramine | M173T199 | C11H14N2 | 11565199.110 | 12992793.690 | 11388819.720 | 0.834 | 0.080 | 0.931 | 0.273 | neg |
| NAD | M662T156 | C21H28N7O14P2 | 1312169.950 | 1327337.900 | 1076027.880 | 0.751 | 0.120 | 0.895 | 0.265 | neg |
| L-Proline | M116T93 | C5H9NO2 | 1314823192.110 | 974295458.520 | 1226165490.880 | 0.309 | 0.510 | 0.940 | 0.262 | pos |
| Dihydrouracil | M114T111 | C4H6N2O2 | 982017.850 | 593015.540 | 818265.440 | 0.587 | 0.230 | 0.834 | 0.260 | neg |
| Sulfamethazine | M279T742 | C12H14N4O2S | 15770326.610 | 17387746.460 | 16169680.170 | 0.523 | 0.280 | 0.940 | 0.260 | pos |
| UDP | M404T72 | C9H14N2O12P2 | 9863945.420 | 12258852.480 | 9826859.040 | 0.960 | 0.020 | 0.976 | 0.257 | neg |
| D-Glucuronic acid | M193T426 | C6H10O7 | 1228138.720 | 1223320.510 | 1204472.350 | 0.834 | 0.080 | 0.931 | 0.255 | neg |
| Pyrophosphate | M177T76 | H4P2O7 | 1371479916.150 | 1921744715.570 | 1665345080.900 | 0.700 | 0.150 | 0.877 | 0.251 | neg |
| L-Isoleucine | M132T295 | C6H13NO2 | 59163705.030 | 63572768.400 | 60228606.000 | 0.849 | 0.070 | 0.963 | 0.243 | pos |
| Hydroxyphenyllactic acid | M181T161_2 | C9H10O4 | 20559613.100 | 18359588.230 | 20919540.510 | 0.884 | 0.050 | 0.948 | 0.240 | neg |
| Diaminopimelic acid | M190T334 | C7H14N2O4 | 8270389.550 | 7873784.570 | 6374375.170 | 0.849 | 0.070 | 0.963 | 0.233 | pos |
| Pyrrole-2-carboxylic acid | M111T735 | C5H5NO2 | 80682955.650 | 89533383.090 | 53286556.680 | 0.504 | 0.300 | 0.940 | 0.230 | pos |
| N-Acetylserotonin | M218T559 | C12H14N2O2 | 53740222.670 | 49029187.630 | 46084837.580 | 0.755 | 0.120 | 0.948 | 0.227 | pos |
| Palmitic acid | M255T839 | C16H32O2 | 21838672.180 | 32543532.800 | 23851017.880 | 0.444 | 0.350 | 0.812 | 0.224 | neg |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Spermidine | M146T66 | C7H19N3 | 225746343.650 | 223025223.570 | 213814634.300 | 0.983 | 0.010 | 0.991 | 0.216 | pos |
| 17a-Estradiol | M271T812 | C18H24O2 | 20869571.930 | 23874239.460 | 20254876.910 | 0.414 | 0.380 | 0.795 | 0.213 | neg |
| Azelaic acid | M187T508 | C9H16O4 | 815268.050 | 775074.770 | 867321.480 | 0.977 | 0.010 | 0.988 | 0.210 | neg |
| N-Acetyl-a-neuraminic acid | M310T107 | C11H19NO9 | 49051020.840 | 70462645.640 | 52047323.200 | 0.529 | 0.280 | 0.940 | 0.197 | pos |
| trans-Aconitic acid | M173T68 | C6H6O6 | 93361292.040 | 108193603.790 | 87761490.220 | 0.911 | 0.040 | 0.961 | 0.196 | neg |
| O-Phosphoethanolamine | M142T84 | C2H8NO4P | 70513472.340 | 70342930.070 | 67431106.330 | 0.834 | 0.080 | 0.963 | 0.189 | pos |
| Sphingosine 1-phosphate | M380T788 | C18H38NO5P | 8557484.620 | 7822136.700 | 6580228.210 | 0.778 | 0.110 | 0.954 | 0.181 | pos |
| Phenylacetylglycine | M192T363 | C10H11NO3 | 9605378.070 | 8532802.700 | 9882593.130 | 0.849 | 0.070 | 0.932 | 0.179 | neg |
| 2-Pyrocatechuic acid | M153T427 | C7H6O4 | 4547996.130 | 3864882.110 | 4538000.550 | 0.645 | 0.190 | 0.861 | 0.160 | neg |
| S-[(E)-N-Hydroxy(indol-3-yl)acetimidoyl]-L-glutathione | M478T70 | C20H25N5O7S | 9899438.190 | 5403048.470 | 6787838.300 | 0.849 | 0.070 | 0.932 | 0.156 | neg |
| 5-Aminopentanoic acid | M116T789 | C5H11NO2 | 4279544.910 | 3328094.920 | 4508541.210 | 0.444 | 0.350 | 0.812 | 0.145 | neg |
| 1,2,3-Trihydroxybenzene | M127T109 | C6H6O3 | 536230588.250 | 543999946.640 | 488157289.700 | 0.805 | 0.090 | 0.954 | 0.138 | pos |
| Caffeate | M180T742 | C9H8O4 | 53480520.350 | 42134420.900 | 53687749.380 | 0.014 | 1.840 | 0.635 | 0.138 | neg |
| Normetanephrine | M166T118 | C9H13NO3 | 45446837.410 | 75875592.460 | 50116070.770 | 0.504 | 0.300 | 0.940 | 0.137 | pos |
| Tryptophanamide | M203T362 | C11H13N3O | 3853094.790 | 10529832.950 | 3627839.700 | 0.011 | 1.950 | 0.635 | 0.132 | neg |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Fumaric acid | M115T72 | C4H4O4 | 273710277.590 | 286113941.430 | 243637442.650 | 0.927 | 0.030 | 0.965 | 0.131 | neg |
| Adenosine | M268T154 | C10H13N5O4 | 386777035.790 | 364929842.130 | 398249179.560 | 0.960 | 0.020 | 0.983 | 0.129 | pos |
| Mannitol | M181T89 | C6H14O6 | 29573242.980 | 29505919.200 | 29625048.680 | 0.932 | 0.030 | 0.965 | 0.101 | neg |
| Betaine | M118T37 | C5H11NO2 | 31799757.410 | 33429628.880 | 29928415.030 | 0.641 | 0.190 | 0.943 | 0.093 | pos |
| N2-gamma-Glutamylglutamine | M274T80 | C10H17N3O6 | 14817993.540 | 53645262.950 | 40525551.400 | 0.949 | 0.020 | 0.976 | 0.084 | neg |
| L-Leucine | M132T172 | C6H13NO2 | 2212350584.300 | 2480669509.150 | 2276117717.750 | 0.700 | 0.150 | 0.947 | 0.076 | pos |
| 16(R)-HETE | M319T839_2 | C20H32O3 | 167717257.170 | 176346623.820 | 180393192.700 | 0.983 | 0.010 | 0.988 | 0.067 | neg |
| 2-Hydroxyadipic acid | M163T115 | C6H10O5 | 20439610.720 | 16067401.590 | 20092972.500 | 0.755 | 0.120 | 0.948 | 0.065 | pos |
| Pipecolic acid | M130T84 | C6H11NO2 | 1197542428.000 | 1411038558.760 | 1165290798.450 | 0.581 | 0.240 | 0.940 | 0.064 | pos |
| Arachidonic acid | M303T839 | C20H32O2 | 45929162.450 | 36021759.330 | 44235476.980 | 0.532 | 0.270 | 0.823 | 0.059 | neg |
| Propionylcarnitine | M218T247 | C10H19NO4 | 37717105.320 | 23274462.000 | 41834565.070 | 0.630 | 0.200 | 0.943 | 0.052 | pos |
| O-Succinyl-L-homoserine | M220T209 | C8H13NO6 | 25110891.960 | 20927118.680 | 32182315.240 | 0.318 | 0.500 | 0.940 | 0.051 | pos |
| L-beta-Phenylalanine | M166T432 | C9H11NO2 | 11456516.320 | 15819696.430 | 10501973.040 | 0.476 | 0.320 | 0.940 | 0.047 | pos |
| epsilon-(gamma-L-Glutamyl)-L-lysine | M275T345_1 | C11H21N3O5 | 12441095.170 | 12930197.890 | 10014435.030 | 0.949 | 0.020 | 0.983 | 0.027 | pos |
| alpha-D-Mannose | M179T243 | C6H12O6 | 12722136.760 | 7079279.030 | 13379030.080 | 0.098 | 1.010 | 0.654 | 0.026 | neg |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Sphingosine | M300T765 | C18H37NO2 | 18592411.120 | 15959848.980 | 18655686.670 | 0.717 | 0.140 | 0.948 | 0.025 | pos |
| Glutaric acid | M131T215 | C5H8O4 | 776197.160 | 1225161.240 | 688483.530 | 0.025 | 1.610 | 0.635 | 0.019 | neg |
| Aspartame | M295T417 | C14H18N2O5 | 26000334.560 | 30920002.060 | 17580427.600 | 0.459 | 0.340 | 0.940 | 0.016 | pos |
| Antibiotic JI-20A | M482T827_2 | C19H39N5O9 | 45663159.570 | 42220604.690 | 56810379.670 | 0.372 | 0.430 | 0.940 | 0.013 | pos |
| 2-Ketobutyric acid | M101T154 | C4H6O3 | 23736346.550 | 35984804.120 | 27065901.110 | 0.359 | 0.440 | 0.778 | 0.001 | neg |

Supplementary table. 4 Screening results of differentially expressed genes

| Gene_name | FC-Con / Q-Con | P value-Con/ Q-Con | FC- Q-Con / T3 | P value- Q-Con / T3 |
|---|---|---|---|---|
| Gja5 | 1.591923139 | 0.005678888 | 0.64405247 | 0.044055728 |
| Acvr1c | 1.63600666 | 0.01757956 | 0.56032091 | 0.029620335 |
| Ankmy1 | 2.058493094 | 0.029391404 | 0.45649196 | 0.037028582 |
| Ap3s1-ps1 | 1.503819765 | 0.035908618 | 0.715874846 | 0.00892305 |
| Appbp2os | 3.068630991 | 0.022191033 | 0.548684663 | 0.049406929 |
| BC046401 | 4.837536196 | 0.005530545 | 0.449219531 | 0.030905764 |
| BC049352 | 1.912624858 | 0.037957299 | 0.398947119 | 0.002352021 |
| Cabp1 | 1.689288756 | 0.008540432 | 0.694938425 | 0.039765915 |
| Ccn4 | 2.112862274 | 0.011340713 | 0.310651065 | 0.001880152 |
| Cd200r4 | 4.093471999 | 0.031998451 | 0.345385359 | 0.025849147 |
| Cdcp1 | 3.909977186 | 0.019269114 | 0.28172652 | 0.01212734 |
| Coch | 1.888142237 | 0.041428628 | 0.529624232 | 0.044295266 |
| Cpne9 | 1.579347709 | 0.006662169 | 0.678793517 | 0.01345094 |
| Csf1r-ps | 9.764876092 | 0.022493972 | 0.121480691 | 0.021522679 |
| Cyb5r4 | 1.729827142 | 0.003588019 | 0.724551471 | 0.029343807 |
| Dach1 | 2.453828821 | 0.021849608 | 0.482434204 | 0.042120035 |
| Egfl8 | 2.257938152 | 0.029398819 | 0.634491024 | 0.046137084 |
| Esd-ps | 2.24963487 | 0.021974281 | 0.522574565 | 0.037922011 |
| Etaa1os | 5.983274693 | 0.01332219 | 0.114344582 | 0.00857367 |
| Fam174b | 1.547065281 | 0.003383086 | 0.675924832 | 0.018695418 |
| Fam180a | 2.331760957 | 0.039243213 | 0.428552285 | 0.011193995 |
| Fam78a | 1.855895999 | 0.006602317 | 0.604017514 | 0.019321063 |
| Fbxo27 | 1.59681897 | 0.012518025 | 0.705398631 | 0.016439099 |
| Fgf14 | 1.629650278 | 0.00529585 | 0.748257709 | 0.045641058 |
| Gabrd | 2.353801662 | 0.005672441 | 0.589736845 | 0.025506233 |
| Gbp6 | 1.901369295 | 0.041664948 | 0.550687784 | 0.0492494 |
| Gdnf | 4.082216328 | 0.030157622 | 0.347465559 | 0.037566546 |
| Htr1b | 1.990854188 | 0.017112769 | 0.633721511 | 0.042720876 |
| Il12rb2 | 2.528078124 | 0.021554704 | 0.418942041 | 0.00983159 |
| Ivns1abp | 1.535014927 | 0.004091161 | 0.747715061 | 0.022279297 |
| Kitl | 2.006838145 | 0.002152094 | 0.659981814 | 0.007627645 |
| Lsmem1 | 4.068512865 | 0.030393359 | 0.288441664 | 0.046803683 |
| Map2k3os | 2.249855961 | 0.018866368 | 0.528078875 | 0.038379137 |
| Map3k8 | 1.577940296 | 0.016632545 | 0.690887038 | 0.020938388 |
| Marchf11 | 1.749038394 | 0.026338637 | 0.700413866 | 0.009504221 |
| Mip | 2.904177737 | 0.008115264 | 0.349415214 | 0.009271812 |
| Myo1b | 1.775290988 | 0.032445312 | 0.646825061 | 0.040930693 |
| Myo1g | 1.754650636 | 0.037531051 | 0.353293065 | 0.03897611 |
| Nexn | 1.90058807 | 0.034511169 | 0.455104936 | 0.02782751 |
| Nup43 | 1.512824524 | 0.042389892 | 0.74869905 | 0.04891432 |
| Papolb | 4.068414908 | 0.011538752 | 0.480051491 | 0.001246573 |
| Pld5 | 2.001885367 | 0.021653773 | 0.538672913 | 0.034142636 |

| | | | | |
|---|---|---|---|---|
| Poln | 2.031508377 | 0.007706957 | 0.626629705 | 0.037489595 |
| Rfc4 | 1.742219794 | 0.006894819 | 0.703087774 | 0.045628822 |
| Rragd | 1.65211977 | 0.009065594 | 0.654718196 | 0.027013606 |
| Runx2os1 | 8.853508271 | 0.030131705 | 0.106562706 | 0.005372332 |
| Scn4b | 2.540196773 | 0.039813294 | 0.397083828 | 0.041064416 |
| Serpinb6b | 1.563466063 | 0.014997478 | 0.579518316 | 0.034084844 |
| Shisa3 | 1.72563533 | 0.034225501 | 0.337937484 | 0.014419258 |
| Slco5a1 | 1.542542699 | 0.005558282 | 0.561963581 | 0.046143199 |
| Slfn2 | 2.131007439 | 0.015687909 | 0.31481327 | 0.008649918 |
| Slfn3 | 4.81558096 | 0.033322427 | 0.272276629 | 0.03136137 |
| Snora61 | 3.112164615 | 0.013261645 | 0.245591052 | 0.013574155 |
| Syndig1 | 1.570985436 | 0.023134479 | 0.72269822 | 0.03522585 |
| Tmem200b | 3.757657128 | 0.017617864 | 0.412094318 | 0.015092915 |
| Vegfc | 1.824806 | 0.041556528 | 0.677772743 | 0.038708647 |
| Zbtb9 | 1.641292456 | 0.008754335 | 0.538665593 | 0.006429115 |
| Zfp114 | 1.504439136 | 0.015181248 | 0.662578967 | 0.004868471 |
| Mir3062 | 7.645576665 | 0.019968105 | 0.257606696 | 0.019135187 |
| Mir3102 | 3.734969409 | 0.042539578 | 0.242190653 | 0.010987219 |
| Mir7045 | 2.32085539 | 0.000467722 | 0.353940406 | 0.035148177 |
| Mir7052 | 1.654357217 | 0.040412222 | 0.652577495 | 0.024355284 |
| Mir760 | 6.858681886 | 0.035604738 | 0.071448513 | 0.021193187 |
| Gramd1c | 0.655583039 | 0.013720148 | 1.672230019 | 0.001942577 |
| Aanat | 0.635492582 | 0.030504487 | 2.179108953 | 0.001073497 |
| Armh1 | 0.44009631 | 0.046147962 | 2.778076057 | 0.025648946 |
| Bub1 | 0.361232292 | 0.023967677 | 2.224953248 | 0.014260609 |
| Cebpd | 0.612072183 | 0.031656973 | 1.75854391 | 0.008011654 |
| Col6a5 | 0.307932258 | 0.017793457 | 2.048825206 | 0.016470868 |
| Dscc1 | 0.161626205 | 0.007203611 | 3.97720369 | 0.008522103 |
| Fam187a | 0.147943506 | 0.004282365 | 3.400610108 | 0.017023056 |
| Foxm1 | 0.652997287 | 0.019133389 | 1.663512443 | 0.005030004 |
| Fscn2 | 0.539834292 | 0.008368405 | 10.20951418 | 0.00394351 |
| Fsip1 | 0.599202516 | 0.029804623 | 1.739098391 | 0.03420539 |
| Gssos1 | 0.160280892 | 0.001976576 | 2.86270736 | 0.006657292 |
| Hgfac | 0.136883024 | 0.023941136 | 18.17146266 | 0.014825851 |
| Hmgb2 | 0.514761898 | 0.049893019 | 1.969562869 | 0.02652935 |
| Hpse2 | 0.117221865 | 0.01237307 | 2.424211574 | 0.043191554 |
| Krt15 | 0.639320355 | 0.046599971 | 2.371086125 | 0.048324486 |
| Maats1 | 0.509615843 | 0.018214656 | 1.731223247 | 0.015225658 |
| Myh13 | 0.511138727 | 0.028501583 | 2.406502514 | 0.019004764 |
| Nek5 | 0.424616161 | 0.017941559 | 2.384115618 | 0.012926524 |
| Nup62cl | 0.158715135 | 0.010604322 | 2.608204227 | 0.044538172 |
| Olfr77 | 0.332899169 | 0.021231899 | 6.677859038 | 0.007789123 |
| Pglyrp2 | 0.383794085 | 0.019574491 | 6.62180069 | 0.039432691 |
| Rpl10-ps2 | 0.482211201 | 0.040147748 | 2.29010744 | 0.011682552 |

| | | | | |
|---|---|---|---|---|
| Slc24a1 | 0.037527703 | 0.033811204 | 3.641325476 | 0.028618609 |
| Slc5a5 | 0.67469092 | 0.014638091 | 1.553810598 | 0.005985222 |
| Smco1 | 0.143196804 | 0.023099114 | 4.662451797 | 0.013189788 |
| Spata3 | 0.3589233 | 0.011654423 | 1.667622213 | 0.02167716 |
| Stap1 | 0.699944338 | 0.008645677 | 1.526790687 | 0.028282561 |
| Tmem236 | 0.530366785 | 0.037910746 | 1.805876171 | 0.051492482 |
| Mir31 | 0.286370323 | 0.006994617 | 6.17747526 | 0.017725693 |
| Mir6943 | 0.158867795 | 0.036158007 | 3.7458131 | 0.008663823 |
| Mir7658 | 0.458717003 | 0.022274245 | 3.001639095 | 0.004432532 |

Supplementary table. 5 Screening the differentially expressed genes in the brain tissues of mice

| gene_name | FC-Con / Q-Con | P value-Con/ Q-Con | FC-Q-Con / T3 | P value-Q-Con/ T3 |
|---|---|---|---|---|
| Bub1 | 0.361232292 | 0.023967677 | 2.224953248 | 0.014260609 |
| Cebpd | 0.612072183 | 0.031656973 | 1.75854391 | 0.008011654 |
| Dscc1 | 0.161626205 | 0.007203611 | 3.97720369 | 0.008522103 |
| Foxm1 | 0.652997287 | 0.019133389 | 1.663512443 | 0.005030004 |
| Hmgb2 | 0.514761898 | 0.049893019 | 1.969562869 | 0.02652935 |
| Nek5 | 0.424616161 | 0.017941559 | 2.384115618 | 0.012926524 |
| Mir31 | 0.286370323 | 0.006994617 | 6.17747526 | 0.017725693 |
| Egfl8 | 2.257938152 | 0.029398819 | 0.634491024 | 0.046137084 |
| Gdnf | 4.082216328 | 0.030157622 | 0.347465559 | 0.037566546 |
| Map3k8 | 1.577940296 | 0.016632545 | 0.690887038 | 0.020938388 |
| Mip | 2.904177737 | 0.008115264 | 0.349415214 | 0.009271812 |
| Myo1b | 1.775290988 | 0.032445312 | 0.646825061 | 0.040930693 |
| Scn4b | 2.540196773 | 0.039813294 | 0.397083828 | 0.041064416 |
| Vegfc | 1.824806 | 0.041556528 | 0.677772743 | 0.038708647 |
| Mir760 | 6.858681886 | 0.035604738 | 0.071448513 | 0.021193187 |
| Fsip1 | 0.599202516 | 0.029804623 | 1.739098391 | 0.03420539 |
| Hpse2 | 0.117221865 | 0.01237307 | 2.424211574 | 0.043191554 |
| Stap1 | 0.699944338 | 0.008645677 | 1.526790687 | 0.028282561 |
| Gja5 | 1.591923139 | 0.005678888 | 0.64405247 | 0.044055728 |
| Cyb5r4 | 1.729827142 | 0.003588019 | 0.724551471 | 0.029343807 |
| Dach1 | 2.453828821 | 0.021849608 | 0.482434204 | 0.042120035 |
| Fgf14 | 1.629650278 | 0.00529585 | 0.748257709 | 0.045641058 |
| Kitl | 2.006838145 | 0.002152094 | 0.659981814 | 0.007627645 |
| Nexn | 1.90058807 | 0.034511169 | 0.455104936 | 0.02782751 |
| Htr1b | 1.990854188 | 0.017112769 | 0.633721511 | 0.042720876 |
| Fbxo27 | 1.59681897 | 0.012518025 | 0.705398631 | 0.016439099 |
| Gabrd | 2.353801662 | 0.005672441 | 0.589736845 | 0.025506233 |
| Map2k3os | 2.249855961 | 0.018866368 | 0.528078875 | 0.038379137 |
| Pld5 | 2.001885367 | 0.021653773 | 0.538672913 | 0.034142636 |
| Rfc4 | 1.742219794 | 0.006894819 | 0.703087774 | 0.045628822 |
| Rragd | 1.65211977 | 0.009065594 | 0.654718196 | 0.027013606 |
| Slfn2 | 2.131007439 | 0.015687909 | 0.31481327 | 0.008649918 |
| Zbtb9 | 1.641292456 | 0.008754335 | 0.538665593 | 0.006429115 |
| Ivns1abp | 1.535014927 | 0.004091161 | 0.747715061 | 0.022279297 |

Supplementary table. 6 Screening results of differentially expressed genes

| gene_name | FC-Con / Q-Con | P value-Con/ Q-Con | FC- Q-Con / T3 | P value- Q-Con / T3 |
|---|---|---|---|---|
| Gja5 | 1.591923139 | 0.005678888 | 0.64405247 | 0.044055728 |
| Acvr1c | 1.63600666 | 0.01757956 | 0.56032091 | 0.029620335 |
| Ankmy1 | 2.058493094 | 0.029391404 | 0.45649196 | 0.037028582 |
| Ap3s1-ps1 | 1.503819765 | 0.035908618 | 0.715874846 | 0.00892305 |
| Appbp2os | 3.068630991 | 0.022191033 | 0.548684663 | 0.049406929 |
| BC046401 | 4.837536196 | 0.005530545 | 0.449219531 | 0.030905764 |
| BC049352 | 1.912624858 | 0.037957299 | 0.398947119 | 0.002352021 |
| Cabp1 | 1.689288756 | 0.008540432 | 0.694938425 | 0.039765915 |
| Ccn4 | 2.112862274 | 0.011340713 | 0.310651065 | 0.001880152 |
| Cd200r4 | 4.093471999 | 0.031998451 | 0.345385359 | 0.025849147 |
| Cdcp1 | 3.909977186 | 0.019269114 | 0.28172652 | 0.01212734 |
| Coch | 1.888142237 | 0.041428628 | 0.529624232 | 0.044295266 |
| Cpne9 | 1.579347709 | 0.006662169 | 0.678793517 | 0.01345094 |
| Csf1r-ps | 9.764876092 | 0.022493972 | 0.121480691 | 0.021522679 |
| Cyb5r4 | 1.729827142 | 0.003588019 | 0.724551471 | 0.029343807 |
| Dach1 | 2.453828821 | 0.021849608 | 0.482434204 | 0.042120035 |
| Egfl8 | 2.257938152 | 0.029398819 | 0.634491024 | 0.046137084 |
| Esd-ps | 2.24963487 | 0.021974281 | 0.522574565 | 0.037922011 |
| Etaa1os | 5.983274693 | 0.01332219 | 0.114344582 | 0.00857367 |
| Fam174b | 1.547065281 | 0.003383086 | 0.675924832 | 0.018695418 |
| Fam180a | 2.331760957 | 0.039243213 | 0.428552285 | 0.011193995 |
| Fam78a | 1.855895999 | 0.006602317 | 0.604017514 | 0.019321063 |
| Fbxo27 | 1.59681897 | 0.012518025 | 0.705398631 | 0.016439099 |
| Fgf14 | 1.629650278 | 0.00529585 | 0.748257709 | 0.045641058 |
| Gabrd | 2.353801662 | 0.005672441 | 0.589736845 | 0.025506233 |
| Gbp6 | 1.901369295 | 0.041664948 | 0.550687784 | 0.0492494 |
| Gdnf | 4.082216328 | 0.030157622 | 0.347465559 | 0.037566546 |
| Htr1b | 1.990854188 | 0.017112769 | 0.633721511 | 0.042720876 |
| Il12rb2 | 2.528078124 | 0.021554704 | 0.418942041 | 0.00983159 |
| Ivns1abp | 1.535014927 | 0.004091161 | 0.747715061 | 0.022279297 |
| Kitl | 2.006838145 | 0.002152094 | 0.659981814 | 0.007627645 |
| Lsmem1 | 4.068512865 | 0.030393359 | 0.288441664 | 0.046803683 |
| Map2k3os | 2.249855961 | 0.018866368 | 0.528078875 | 0.038379137 |
| Map3k8 | 1.577940296 | 0.016632545 | 0.690887038 | 0.020938388 |
| Marchf11 | 1.749038394 | 0.026338637 | 0.700413866 | 0.009504221 |
| Mip | 2.904177737 | 0.008115264 | 0.349415214 | 0.009271812 |
| Myo1b | 1.775290988 | 0.032445312 | 0.646825061 | 0.040930693 |
| Myo1g | 1.754650636 | 0.037531051 | 0.353293065 | 0.03897611 |
| Nexn | 1.90058807 | 0.034511169 | 0.455104936 | 0.02782751 |
| Nup43 | 1.512824524 | 0.042389892 | 0.74869905 | 0.04891432 |
| Papolb | 4.068414908 | 0.011538752 | 0.480051491 | 0.001246573 |
| Pld5 | 2.001885367 | 0.021653773 | 0.538672913 | 0.034142636 |

| | | | | |
|---|---|---|---|---|
| Poln | 2.031508377 | 0.007706957 | 0.626629705 | 0.037489595 |
| Rfc4 | 1.742219794 | 0.006894819 | 0.703087774 | 0.045628822 |
| Rragd | 1.65211977 | 0.009065594 | 0.654718196 | 0.027013606 |
| Runx2os1 | 8.853508271 | 0.030131705 | 0.106562706 | 0.005372332 |
| Scn4b | 2.540196773 | 0.039813294 | 0.397083828 | 0.041064416 |
| Serpinb6b | 1.563466063 | 0.014997478 | 0.579518316 | 0.034084844 |
| Shisa3 | 1.72563533 | 0.034225501 | 0.337937484 | 0.014419258 |
| Slco5a1 | 1.542542699 | 0.005558282 | 0.561963581 | 0.046143199 |
| Slfn2 | 2.131007439 | 0.015687909 | 0.31481327 | 0.008649918 |
| Slfn3 | 4.81558096 | 0.033322427 | 0.272276629 | 0.03136137 |
| Snora61 | 3.112164615 | 0.013261645 | 0.245591052 | 0.013574155 |
| Syndig1 | 1.570985436 | 0.023134479 | 0.72269822 | 0.03522585 |
| Tmem200b | 3.757657128 | 0.017617864 | 0.412094318 | 0.015092915 |
| Vegfc | 1.824806 | 0.041556528 | 0.677772743 | 0.038708647 |
| Zbtb9 | 1.641292456 | 0.008754335 | 0.538665593 | 0.006429115 |
| Zfp114 | 1.504439136 | 0.015181248 | 0.662578967 | 0.004868471 |
| Mir3062 | 7.645576665 | 0.019968105 | 0.257606696 | 0.019135187 |
| Mir3102 | 3.734969409 | 0.042539578 | 0.242190653 | 0.010987219 |
| Mir7045 | 2.32085539 | 0.000467722 | 0.353940406 | 0.035148177 |
| Mir7052 | 1.654357217 | 0.040412222 | 0.652577495 | 0.024355284 |
| Mir760 | 6.858681886 | 0.035604738 | 0.071448513 | 0.021193187 |
| Gramd1c | 0.655583039 | 0.013720148 | 1.672230019 | 0.001942577 |
| Aanat | 0.635492582 | 0.030504487 | 2.179108953 | 0.001073497 |
| Armh1 | 0.44009631 | 0.046147962 | 2.778076057 | 0.025648946 |
| Bub1 | 0.361232292 | 0.023967677 | 2.224953248 | 0.014260609 |
| Cebpd | 0.612072183 | 0.031656973 | 1.75854391 | 0.008011654 |
| Col6a5 | 0.307932258 | 0.017793457 | 2.048825206 | 0.016470868 |
| Dscc1 | 0.161626205 | 0.007203611 | 3.97720369 | 0.008522103 |
| Fam187a | 0.147943506 | 0.004282365 | 3.400610108 | 0.017023056 |
| Foxm1 | 0.652997287 | 0.019133389 | 1.663512443 | 0.005030004 |
| Fscn2 | 0.539834292 | 0.008368405 | 10.20951418 | 0.00394351 |
| Fsip1 | 0.599202516 | 0.029804623 | 1.739098391 | 0.03420539 |
| Gssos1 | 0.160280892 | 0.001976576 | 2.86270736 | 0.006657292 |
| Hgfac | 0.136883024 | 0.023941136 | 18.17146266 | 0.014825851 |
| Hmgb2 | 0.514761898 | 0.049893019 | 1.969562869 | 0.02652935 |
| Hpse2 | 0.117221865 | 0.01237307 | 2.424211574 | 0.043191554 |
| Krt15 | 0.639320355 | 0.046599971 | 2.371086125 | 0.048324486 |
| Maats1 | 0.509615843 | 0.018214656 | 1.731223247 | 0.015225658 |
| Myh13 | 0.511138727 | 0.028501583 | 2.406502514 | 0.019004764 |
| Nek5 | 0.424616161 | 0.017941559 | 2.384115618 | 0.012926524 |
| Nup62cl | 0.158715135 | 0.010604322 | 2.608204227 | 0.044538172 |
| Olfr77 | 0.332899169 | 0.021231899 | 6.677859038 | 0.007789123 |
| Pglyrp2 | 0.383794085 | 0.019574491 | 6.62180069 | 0.039432691 |
| Rpl10-ps2 | 0.482211201 | 0.040147748 | 2.29010744 | 0.011682552 |

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|---|---|---|---|---|
| Slc24a1 | 0.037527703 | 0.033811204 | 3.641325476 | 0.028618609 |
| Slc5a5 | 0.67469092 | 0.014638091 | 1.553810598 | 0.005985222 |
| Smco1 | 0.143196804 | 0.023099114 | 4.662451797 | 0.013189788 |
| Spata3 | 0.3589233 | 0.011654423 | 1.667622213 | 0.02167716 |
| Stap1 | 0.699944338 | 0.008645677 | 1.526790687 | 0.028282561 |
| Tmem236 | 0.530366785 | 0.037910746 | 1.805876171 | 0.051492482 |
| Mir31 | 0.286370323 | 0.006994617 | 6.17747526 | 0.017725693 |
| Mir6943 | 0.158867795 | 0.036158007 | 3.7458131 | 0.008663823 |
| Mir7658 | 0.458717003 | 0.022274245 | 3.001639095 | 0.004432532 |

Supplementary table. 7 The KEGG information of differentially expressed genes

| KEGG ID | Term description | Observed gene count | Background gene count | Strength | False discovery rate | Matching proteins in your network (labels) |
|---|---|---|---|---|---|---|
| mmu04620 | Toll-like receptor signaling pathway | 7 | 98 | 1.2000 | 0.0002 | Traf6, Cd40, Tbk1, Traf3, Tab1, Map3k8, Irf7 |
| mmu04622 | RIG-I-like receptor signaling pathway | 4 | 70 | 1.1000 | 0.0113 | Traf6, Tbk1, Traf3, Irf7 |
| mmu04064 | NF-kappa B signaling pathway | 5 | 99 | 1.0500 | 0.0069 | Traf6,Birc3,Cd40,Traf3,Tab1 |
| mmu04668 | TNF signaling pathway | 5 | 112 | 1.0000 | 0.0075 | Birc3, Traf3, Tab1, Map3k8, Vegfc |
| mmu05161 | Hepatitis B | 6 | 161 | 0.9200 | 0.0069 | Traf6,Tbk1,Grb2,Traf3,Tab1,Irf7 |
| mmu05145 | Toxoplasmosis | 4 | 106 | 0.9200 | 0.0358 | Traf6, Birc3, Cd40, Tab1 |
| mmu04114 | Oocyte meiosis | 4 | 115 | 0.8900 | 0.0445 | Cdc20, Fbxo5, Cdk1, Bub1 |
| mmu05160 | Hepatitis C | 5 | 158 | 0.8500 | 0.0230 | Traf6,Tbk1,Grb2,Traf3,Irf7 |
| mmu04010 | MAPK signaling pathway | 9 | 289 | 0.8400 | 0.0013 | Ngfr, Traf6, Kit, Flt4, Grb2, Tab1, Map3k8, Vegfc, Kitl |
| mmu04014 | Ras signaling pathway | 7 | 224 | 0.8400 | 0.0067 | Ngfr, Kit, Tbk1, Flt4, Grb2, Vegfc, Kitl |
| mmu04621 | NOD-like receptor signaling pathway | 6 | 191 | 0.8400 | 0.0096 | Traf6, Birc3, Tbk1, Traf3, Tab1, Irf7 |
| mmu04060 | Cytokine-cytokine receptor interaction | 8 | 279 | 0.8100 | 0.0049 | Ngfr, Il12rb1, Il12rb2, Cd40, Gdf11, Acvr1c, Gdf3, Acvr2b |
| mmu05169 | Epstein-Barr virus infection | 6 | 214 | 0.8000 | 0.0141 | Traf6, Cd40, Tbk1, Traf3, Tab1, Irf7 |
| mmu05203 | Viral carcinogenesis | 5 | 194 | 0.7600 | 0.0445 | Cdc20, Cdk1, Grb2, Traf3, Irf7 |
| mmu04510 | Focal adhesion | 5 | 196 | 0.7500 | 0.0445 | Birc3, Flt4, Grb2, Vegfc, Col6a5 |
| mmu04015 | Rap1 signaling pathway | 5 | 208 | 0.7300 | 0.0498 | Ngfr, Kit, Flt4, Vegfc, Kitl |
| mmu04151 | PI3K-Akt signaling pathway | 7 | 355 | 0.6400 | 0.0309 | Ngfr, Kit, Flt4, Grb2, Vegfc, Kitl, Col6a5 |
| mmu05200 | Pathways in cancer | 10 | 528 | 0.6300 | 0.0070 | Il12rb1, Traf6, Kit, Il12rb2, Birc3, Flt4, Grb2, Traf3, Vegfc, Kitl |
| mmu05168 | Herpes simplex virus 1 infection | 7 | 413 | 0.5800 | 0.0498 | Traf6, Birc3, Tbk1, Traf3, Tab1, Irf7, Zfp114 |