

S3 Table. Metabolome data for the livers of irradiated mice administered sake. Values represent the relative areas of each metabolite peak to the peak area of an internal standard.

| Compound name | Relative Area | | | | | | | | | | | | Comparative Analysis | | | | | | | | | | | | | | | | | | | |
|------------------------------------|---------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|----------------------|---------|---------|---------|-----------------|---------|---------|---------|--------------------|-----------------------|--------------------|-----------------------|--------------------|-----------------------|--------------------|-----------------------|--------------------|-----------------------|-------|----|
| | control | | | | rad | | | | sake | | | | sake+rad | | | | sake vs control | | | | sake+rad vs rad | | | | sake+rad vs sake | | | | | | | |
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | Mean | S.D. | Mean | S.D. | Mean | S.D. | Mean | S.D. | Ratio ¹ | p-value ^{II} | Ratio ¹ | p-value ^{II} | Ratio ¹ | p-value ^{II} | Ratio ¹ | p-value ^{II} | Ratio ¹ | p-value ^{II} | | |
| Oxotanic acid | N.D. | N.D. | N.D. | N.D. | 1.3E-04 | N.D. | 3.8E-04 | 5.4E-04 | 4.2E-04 | N.D. | N.D. | N.D. | N.A. | 1.3E-04 | N.A. | 4.4E-04 | 8.7E-05 | N.D. | N.A. | N.A. | <1 | N.A. | <1 | N.A. | N.A. | N.A. | <1 | N.A. | <1 | N.A. | | |
| XA0013 | N.D. | N.D. | N.D. | 1.7E-04 | N.D. | N.D. | N.D. | 4.6E-04 | N.D. | N.D. | N.D. | N.D. | N.A. | 1.7E-04 | N.A. | 4.6E-04 | N.A. | N.A. | N.A. | N.A. | <1 | N.A. | <1 | N.A. | N.A. | N.A. | <1 | N.A. | <1 | N.A. | | |
| Fructose 1,6-diphosphate | 2.9E-04 | 3.6E-04 | 3.1E-04 | 3.2E-03 | 4.9E-04 | 3.8E-04 | 3.1E-04 | 2.8E-04 | 2.8E-04 | 2.7E-04 | 3.7E-04 | 3.8E-04 | 3.2E-04 | 3.8E-05 | 1.4E-03 | 1.6E-03 | 2.9E-04 | 1.8E-05 | 3.4E-04 | 6.2E-05 | 4.2 | 0.378 | 1.1 | 0.713 | 0.2 | 0.385 | 1.2 | 0.325 | | | | |
| UDP-glucose | 2.5E-04 | 2.4E-04 | 4.7E-04 | 2.0E-03 | 6.2E-04 | 3.9E-04 | N.D. | 3.0E-04 | 1.6E-04 | 8.5E-04 | 6.0E-04 | 3.2E-04 | 1.3E-05 | 1.0E-05 | 9.9E-05 | 8.5E-05 | 2.7E-04 | 4.2E-05 | 5.4E-04 | 3.5E-04 | 3.1 | 0.308 | 1.7 | 0.403 | 0.5 | 0.464 | 2.0 | 0.315 | | | | |
| UDP-galactose | 7.8E-03 | 1.1E-02 | 1.4E-02 | 2.4E-02 | 2.9E-02 | 3.6E-02 | 9.5E-03 | 8.9E-03 | 1.2E-02 | 1.9E-02 | 1.8E-02 | 1.1E-02 | 3.2E-03 | 3.0E-02 | 6.1E-03 | 1.0E-02 | 1.6E-03 | 1.8E-02 | 1.5E-03 | 2.7 | 0.018 | 0.9 | 0.743 | 1.6 | 0.047 | 0.6 | 0.072 | 1.8 | 0.004 | ** | | |
| Tauricholic acid | 4.6E-02 | 4.1E-02 | 3.3E-02 | 1.2E-01 | 4.9E-02 | 5.0E-02 | 7.5E-02 | 4.7E-02 | 1.6E-02 | 3.0E-02 | 4.6E-02 | 6.8E-02 | 3.3E-02 | 4.0E-02 | 6.6E-02 | 4.9E-02 | 2.6E-02 | 3.2E-02 | 4.1E-02 | 2.1 | 0.158 | 0.8 | 0.428 | 0.4 | 0.106 | 0.6 | 0.382 | | | | | |
| 3'-ADP | 2.3E-04 | 2.5E-04 | 2.6E-04 | 3.9E-04 | 3.5E-04 | 6.7E-04 | 2.3E-04 | 2.3E-04 | 2.6E-04 | 1.9E-04 | 1.8E-04 | 1.5E-04 | 2.5E-04 | 1.6E-05 | 4.7E-04 | 1.7E-04 | 2.4E-04 | 1.8E-05 | 1.7E-04 | 2.2E-05 | 1.9 | 0.154 | 1.0 | 0.629 | 0.7 | 0.011 | 0.4 | 0.093 | 0.7 | 0.015 | * | |
| Dihydroxyacetone phosphate | 2.1E-03 | 2.4E-03 | 3.8E-03 | 9.4E-03 | 4.2E-03 | 3.5E-03 | 1.7E-03 | 2.6E-03 | 1.2E-03 | 1.7E-03 | 2.8E-03 | 2.8E-03 | 4.7E-03 | 2.8E-03 | 6.8E-03 | 4.2E-03 | 4.6E-03 | 2.9E-03 | 2.1E-03 | 1.9 | 0.380 | 1.0 | 0.930 | 3.0 | 0.6 | 0.407 | 1.3 | 0.588 | | | | |
| S | 2.0E-04 | 1.4E-04 | 1.7E-04 | 2.3E-04 | 1.8E-04 | 4.8E-04 | 2.2E-04 | 2.6E-04 | 7.2E-04 | 1.6E-04 | 4.1E-04 | 2.2E-04 | 1.7E-04 | 2.8E-05 | 3.0E-04 | 1.6E-04 | 4.0E-04 | 2.7E-04 | 2.6E-04 | 1.3E-04 | 1.8 | 0.298 | 2.4 | 0.277 | 1.6 | 0.336 | 0.9 | 0.793 | 0.7 | 0.493 | | |
| Lactoylglutathione | 4.9E-02 | 5.6E-02 | 8.2E-02 | 7.5E-02 | 1.1E-01 | 1.3E-01 | 5.2E-02 | 6.8E-02 | 7.9E-02 | 9.5E-02 | 1.3E-02 | 1.1E-01 | 6.3E-02 | 1.8E-02 | 1.1E-01 | 3.0E-02 | 6.6E-02 | 1.3E-02 | 9.8E-02 | 6.4E-03 | 1.7 | 0.111 | 1.0 | 0.827 | 1.6 | 0.059 | 0.9 | 0.698 | 1.5 | 0.035 | * | |
| Tetrahydrobiopterin | N.D. | N.D. | 1.2E-04 | N.D. | 1.9E-04 | N.D. | N.D. | 1.9E-04 | N.D. | 1.1E-04 | 1.4E-04 | 1.2E-04 | 1.2E-04 | N.A. | 1.9E-04 | N.A. | 1.1E-04 | N.A. | 1.3E-04 | 9.8E-06 | 1.7 | N.A. | 1.0 | N.A. | 1.1 | N.A. | 0.7 | N.A. | 1.2 | N.A. | | |
| Triethanolamine | 6.0E-05 | 7.4E-05 | 6.4E-05 | 1.4E-04 | 1.1E-04 | 6.7E-05 | 8.5E-04 | 6.4E-05 | 7.4E-05 | 6.1E-05 | 5.6E-05 | 9.0E-05 | 6.6E-05 | 7.5E-06 | 1.1E-04 | 3.7E-05 | 3.3E-04 | 4.5E-06 | 6.9E-05 | 1.8E-05 | 1.6 | 0.191 | 1.0 | 0.813 | 0.6 | 0.211 | 0.2 | 0.423 | | | | |
| γ-Glu-2-aminobutyric acid | 1.5E-04 | 1.5E-04 | 2.3E-04 | 2.3E-04 | 3.2E-04 | 3.1E-04 | 1.8E-04 | 1.6E-04 | 1.5E-04 | 1.7E-04 | 1.9E-04 | 2.0E-04 | 1.8E-04 | 1.4E-05 | 2.9E-04 | 5.0E-05 | 1.6E-04 | 1.2E-05 | 1.9E-04 | 1.4E-05 | 1.6 | 0.053 | 0.9 | 0.665 | 1.1 | 0.723 | 0.7 | 0.071 | 1.2 | 0.074 | | |
| Cys | 1.6E-04 | 1.3E-04 | 1.4E-04 | 2.0E-04 | 2.2E-04 | 2.6E-04 | 1.5E-04 | 2.4E-04 | 2.3E-04 | 4.2E-04 | 4.5E-04 | 4.0E-04 | 1.4E-04 | 1.8E-05 | 2.3E-04 | 2.1E-04 | 4.7E-04 | 4.2E-04 | 2.9E-05 | 1.6 | 0.014 | 1.4 | 0.129 | 3.0 | 4.1E-04 | *** | 1.9 | 0.001 | ** | | | |
| Inosine | 2.0E-02 | 2.0E-02 | 2.5E-02 | 4.2E-02 | 3.1E-02 | 2.9E-02 | 2.3E-02 | 2.6E-02 | 3.2E-02 | 4.1E-02 | 3.2E-02 | 2.1E-02 | 2.7E-03 | 3.4E-02 | 6.8E-03 | 2.7E-02 | 4.5E-03 | 3.6E-02 | 4.6E-03 | 1.6 | 0.070 | 1.7 | 0.015 | 1.1 | 0.699 | 1.3 | 0.078 | | | | | |
| Phosphoenolpyruvic acid | 4.6E-04 | 5.4E-04 | 6.8E-04 | 8.5E-04 | 8.7E-04 | 9.6E-04 | 3.8E-04 | 4.5E-04 | 4.0E-04 | 5.7E-04 | 5.3E-04 | 7.5E-04 | 6.6E-04 | 1.1E-04 | 8.7E-04 | 2.7E-05 | 4.1E-04 | 3.7E-05 | 6.1E-04 | 1.2E-04 | 1.6 | 0.033 | 0.7 | 0.131 | 1.1 | 0.608 | 0.7 | 0.063 | 1.5 | 0.094 | | |
| Creatine | 3.2E-02 | 3.0E-02 | 2.8E-02 | 4.4E-02 | 4.9E-02 | 4.6E-02 | 2.5E-02 | 2.5E-02 | 2.6E-02 | 5.0E-02 | 3.2E-02 | 3.0E-02 | 1.9E-03 | 4.6E-02 | 2.7E-03 | 2.5E-02 | 4.4E-04 | 4.0E-02 | 8.3E-03 | 1.5 | 0.020 | ** | 0.8 | 0.044 | 1.3 | 0.156 | 0.9 | 0.345 | 1.6 | 0.087 | | |
| 3-Phosphoglyceric acid | 1.0E-03 | 1.2E-03 | 1.4E-03 | 1.8E-03 | 1.7E-03 | 1.2E-03 | 6.9E-04 | 9.2E-04 | 8.7E-04 | 1.2E-03 | 1.6E-03 | 1.2E-03 | 2.0E-04 | 1.9E-03 | 2.2E-04 | 8.3E-04 | 1.3E-03 | 2.1E-04 | 1.5 | 0.002 | ** | 0.7 | 0.053 | 1.1 | 0.550 | 0.7 | 0.041 | 1.6 | 0.036 | ** | | |
| XA0035 | 4.3E-04 | 4.3E-04 | 4.4E-04 | 5.7E-04 | 6.3E-04 | 7.5E-04 | 3.1E-04 | 4.1E-04 | 4.5E-04 | 5.4E-04 | 5.1E-04 | 4.2E-04 | 3.4E-04 | 7.0E-06 | 6.5E-04 | 9.1E-05 | 3.8E-04 | 6.0E-05 | 4.9E-04 | 6.0E-05 | 1.5 | 0.055 | 0.9 | 0.260 | 1.1 | 0.244 | 0.8 | 0.078 | 1.3 | 0.088 | | |
| Homovanillic acid | 1.6E-04 | 2.4E-04 | 2.0E-04 | 1.5E-04 | 4.2E-04 | 3.1E-04 | 2.4E-04 | 2.0E-04 | 2.2E-04 | 3.2E-04 | 1.9E-04 | 2.0E-04 | 4.0E-05 | 2.9E-04 | 4.1E-05 | 2.1E-04 | 2.2E-05 | 2.7E-04 | 6.7E-05 | 1.5 | 0.392 | 1.1 | 0.833 | 1.4 | 0.217 | 0.9 | 0.806 | 1.3 | 0.283 | | | |
| Ascorbic acid | 1.6E-02 | 2.0E-02 | 2.3E-02 | 2.0E-02 | 2.8E-02 | 3.6E-02 | 1.5E-02 | 1.7E-02 | 2.7E-02 | 3.8E-02 | 3.1E-02 | 2.8E-02 | 1.9E-02 | 3.7E-03 | 2.8E-02 | 7.5E-03 | 2.0E-02 | 6.9E-03 | 3.2E-02 | 3.8E-03 | 1.4 | 0.184 | 1.0 | 0.936 | 1.6 | 0.017 | 1.1 | 0.510 | 1.6 | 0.072 | | |
| 3-Deoxyphospho-N-acetylglucosamine | 1.8E-04 | 1.2E-04 | 1.7E-04 | 2.0E-04 | 2.0E-04 | 2.8E-04 | 1.6E-04 | 2.0E-04 | 2.7E-04 | 4.8E-04 | 4.8E-04 | 1.6E-04 | 3.3E-05 | 2.2E-04 | 4.8E-05 | 2.1E-04 | 5.7E-05 | 4.4E-04 | 5.7E-05 | 1.4 | 0.124 | 1.3 | 0.248 | 2.8 | 0.004 | ** | 2.0 | 0.008 | ** | 2.1 | 0.007 | ** |
| Acetylglucosamine | 3.8E-04 | 4.4E-04 | 5.5E-04 | 5.4E-04 | 5.1E-04 | 8.7E-04 | 4.2E-04 | 4.2E-04 | 5.8E-04 | 3.9E-04 | 5.3E-04 | 4.6E-04 | 8.6E-05 | 6.4E-04 | 2.0E-04 | 4.1E-04 | 8.4E-05 | 4.3E-04 | 4.7E-05 | 1.4 | 0.255 | 0.9 | 0.457 | 1.2 | 0.278 | 0.8 | 0.458 | 1.3 | 0.044 | ** | | |
| Diphosphoglyceric acid | 5.8E-03 | 7.9E-03 | 4.9E-03 | 1.3E-02 | 6.7E-03 | 5.9E-03 | 6.2E-03 | 5.9E-03 | 4.2E-03 | 5.1E-03 | 5.8E-03 | 5.9E-03 | 6.1E-03 | 1.6E-03 | 8.5E-03 | 3.9E-03 | 5.4E-03 | 1.1E-03 | 5.5E-03 | 4.0E-04 | 1.4 | 0.405 | 0.9 | 0.543 | 0.9 | 0.574 | 0.6 | 0.312 | 1.0 | 0.861 | | |
| 5-Choroline | 6.3E-04 | 4.4E-04 | 4.9E-04 | 9.8E-04 | 5.8E-04 | 6.0E-04 | 7.7E-04 | 5.7E-04 | 5.5E-04 | 8.7E-04 | 7.7E-04 | 7.5E-04 | 5.2E-04 | 9.8E-05 | 7.2E-04 | 2.3E-04 | 6.3E-04 | 1.2E-04 | 8.0E-04 | 6.5E-05 | 1.4 | 0.284 | 1.2 | 0.280 | 1.5 | 0.019 | * | 1.1 | 0.813 | 1.3 | 0.116 | |
| Ribulose 5-phosphate | 6.0E-03 | 5.8E-03 | 6.2E-03 | 9.4E-03 | 6.8E-03 | 8.2E-03 | 5.9E-03 | 6.2E-03 | 6.2E-03 | 8.8E-03 | 7.7E-03 | 7.8E-03 | 6.0E-03 | 8.1E-03 | 1.3E-03 | 6.2E-03 | 3.1E-04 | 8.1E-03 | 6.8E-04 | 1.4 | 0.100 | 1.0 | 0.337 | 1.3 | 0.027 | ** | 1.0 | 0.954 | 1.3 | 0.027 | * | |
| Fructose 6-phosphate | 6.7E-03 | 4.9E-03 | 6.9E-03 | 1.2E-02 | 6.3E-03 | 6.7E-03 | 6.5E-03 | 7.2E-03 | 6.9E-03 | 6.0E-03 | 2.6E-03 | 6.0E-03 | 4.2E-03 | 6.2E-03 | 1.1E-03 | 8.4E-03 | 3.1E-03 | 6.8E-03 | 3.5E-04 | 1.7E-03 | 1.4 | 0.356 | 1.1 | 0.410 | 0.7 | 0.193 | 0.5 | 0.140 | 0.6 | 0.119 | | |
| Adenosine | 2.8E-02 | 3.0E-02 | 2.9E-02 | 2.7E-02 | 4.2E-02 | 4.7E-02 | 2.7E-02 | 2.4E-02 | 3.5E-02 | 2.9E-02 | 2.9E-02 | 2.9E-02 | 2.9E-02 | 1.1E-02 | 2.2E-02 | 5.1E-03 | 2.9E-02 | 5.1E-03 | 1.3 | 0.260 | 0.8 | 0.148 | 1.0 | 0.899 | 0.8 | 0.277 | 1.3 | 0.163 | | | | |
| XC0126 | 1.8E-04 | 1.4E-04 | 1.4E-04 | 1.7E-04 | 1.7E-04 | 2.6E-04 | 1.4E-04 | 1.5E-04 | 1.7E-04 | 2.3E-04 | 2.0E-04 | 1.7E-04 | 1.6E-04 | 2.3E-05 | 2.0E-04 | 5.0E-05 | 1.8E-05 | 2.0E-04 | 3.0E-05 | 1.3 | 0.283 | 1.3 | 0.141 | 1.0 | 0.839 | 1.0 | 0.919 | 1.3 | 0.108 | | | |
| Gln | 3.5E-01 | 2.3E-01 | 2.8E-01 | 3.5E-01 | 2.6E-01 | 2.8E-01 | 2.1E-01 | 2.4E-01 | 2.1E-01 | 2.1E-01 | 2.7E-01 | 2.8E-01 | 2.6E-01 | 2.3E-01 | 1.7E-02 | 3.0E-01 | 4.4E-02 | 2.2E-01 | 1.7E-02 | 0.9 | 0.302 | 1.1 | 0.082 | 1.1 | 0.092 | 1.1 | 0.092 | 1.2 | 0.092 | | | |
| Hexanoic acid | 2.4E-04 | N.D. | 2.4E-04 | N.D. | 3.0E-04 | N.D. | 4.6E-04 | 9.1E-04 | 5.6E-04 | 3.0E-04 | 2.5E-04 | N.D. | 2.4E-04 | 4.3E-06 | 3.0E-04 | N.A. | 6.4E-04 | 2.4E-04 | 2.8E-04 | 3.1E-05 | 1.3 | N.A. | 2.7 | 0.099 | 1.2 | 0.384 | 0.9 | N.A. | 0.4 | 0.112 | | |
| γ-Aminobutyric acid | 3.4E-03 | 4.2E-03 | 4.2E-03 | 7.4E-03 | 4.9E-03 | 2.4E-03 | 5.5E-03 | 6.1E-03 | 9.0E-03 | 5.1E-03 | 6.9E-03 | 7.2E-03 | 6.3E-03 | 4.6E-04 | 5.9E-03 | 2.5E-03 | 3.9E-04 | 7.7E-03 | 3.6E-03 | 1.2 | 0.574 | 2.0 | 0.017 | 1.6 | 0.182 | 1.4 | 0.061 | | | | | |
| N ⁶ -acetyllysine | 6.1E-04 | 5.4E-04 | 6.5E-04 | 8.0E-04 | 6.7E-04 | 7.7E-04 | 5.8E-04 | 6.4E-04 | 4.9E-04 | 7.2E-04 | 5.6E-04 | 6.2E-04 | 6.0E-04 | 5.5E-05 | 7.5E-04 | 6.7E-05 | 5.7E-04 | 7.7E-05 | 6.4E-04 | 7.1E-05 | 1.2 | 0.043 | 1.0 | 0.628 | 1.1 | 0.450 | 0.9 | 0.136 | 1.1 | 0.286 | | |
| CoA-divalent glutathione | 5.5E-03 | 4.2E-03 | 6.2E-03 | 5.9E-03 | 6.1E-03 | 7.6E-03 | 5.1E-03 | 6.3E-03 | 7.1E-03 | 6.0E-03 | 6.3E-03 | 7.3E-03 | 6.9E-03 | 9.9E-04 | 6.6E-03 | 9.4E-04 | 6.6E-03 | 1.0E-03 | 7.7E-03 | 4.5E-04 | 1.2 | 0.183 | 1.2 | 0.356 | 1.5 | 0.035 | 1.2 | 0.150 | 1.3 | 0.092 | | |
| Nitrate | 3.8E-01 | 3.4E-01 | 4.5E-01 | 4.5E-01 | 4.5E-01 | 4.1E-01 | 4.0E-01 | 4.0E-01 | 5.8E-01 | 3.9E-01 | 5.8E-01 | 5.8E-01 | 4.8E-01 | 3.4E-02 | 4.3E-01 | 5.9E-02 | 5.9E-01 | 4.1E-02 | 1.2 | 0.082 | 1.1 | 0.082 | 1.1 | 0.082 | 1.1 | 0.082 | 1.1 | 0.082 | | | | |
| Lactic acid | 4.0E-01 | 4.0E-01 | 4.8E-01 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----------------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|----------|---------|---------|---------|-------|-------|-------|-------|-------|-------|-------|-------|---------|-------|-------|-------|
| XAD019 | 4.9E-03 | 2.7E-03 | 2.6E-03 | 2.3E-03 | 5.1E-03 | 3.4E-03 | 3.1E-03 | 3.7E-03 | 2.7E-03 | 2.7E-03 | 2.9E-03 | 3.3E-03 | 3.4E-03 | 1.3E-03 | 3.6E-03 | 1.4E-03 | 3.1E-03 | 4.7E-04 | 2.8E-03 | 4.4E-04 | 1.1 | 0.856 | 0.9 | 0.778 | 0.8 | 0.529 | 0.8 | 0.451 | 0.9 | 0.437 | | | |
| Cytidine | 3.9E-04 | 6.2E-04 | 3.7E-04 | 3.9E-04 | 4.2E-04 | 3.9E-04 | 3.9E-04 | 3.9E-04 | 3.9E-04 | 3.9E-04 | 3.9E-04 | 3.9E-04 | 3.9E-04 | 3.9E-04 | 3.9E-04 | 3.9E-04 | 3.9E-04 | 3.9E-04 | 3.9E-04 | 3.9E-04 | 3.9E-04 | 1.1 | 0.707 | 1.1 | 0.565 | 1.1 | 0.722 | 1.1 | 0.228 | 1.1 | 0.278 | | |
| CDP-uridine | 4.2E-04 | 5.6E-04 | 4.8E-04 | 3.3E-04 | 5.7E-04 | 6.4E-04 | 6.1E-04 | 5.6E-04 | 4.3E-04 | 5.1E-04 | 4.7E-04 | 5.0E-04 | 4.8E-04 | 7.1E-05 | 5.1E-04 | 1.6E-04 | 5.3E-04 | 0.97E-05 | 4.9E-04 | 3.2E-05 | 1.1 | 0.815 | 1.1 | 0.532 | 1.0 | 0.875 | 1.0 | 0.860 | 0.9 | 0.550 | | | |
| Choline | 3.7E-03 | 4.1E-03 | 4.0E-03 | 4.2E-03 | 4.2E-03 | 4.1E-03 | 4.5E-03 | 5.4E-03 | 4.4E-03 | 4.7E-03 | 5.0E-03 | 3.9E-03 | 2.2E-04 | 4.2E-03 | 2.5E-03 | 4.8E-03 | 5.3E-04 | 4.5E-04 | 3.0E-04 | 1.1 | 0.242 | 1.2 | 0.102 | 1.3 | 0.006 | ** | 1.2 | 0.028 | * | 1.1 | 0.348 | | |
| AMP | 7.5E-04 | 8.9E-04 | 7.0E-04 | 5.6E-04 | 9.2E-04 | 8.1E-04 | 7.9E-04 | 7.4E-04 | 1.1E-03 | 1.1E-03 | 1.0E-03 | 7.8E-04 | 1.0E-04 | 8.2E-04 | 2.2E-04 | 7.8E-04 | 3.4E-05 | 1.0E-03 | 3.3E-05 | 1.1 | 0.798 | 1.0 | 0.992 | 1.3 | 0.034 | ** | 1.3 | 0.224 | 1.3 | 6.7E-04 | *** | | |
| TP | 8.2E-03 | 7.9E-03 | 5.2E-03 | 7.6E-03 | 8.0E-03 | 6.7E-03 | 6.9E-03 | 7.8E-03 | 7.6E-03 | 6.5E-03 | 6.5E-03 | 7.1E-03 | 1.6E-03 | 7.4E-03 | 7.1E-04 | 7.1E-03 | 4.2E-04 | 6.5E-03 | 1.1E-03 | 1.1 | 0.755 | 1.0 | 0.976 | 1.0 | 0.976 | 0.9 | 0.650 | 0.9 | 0.285 | 0.9 | 0.439 | | |
| ClA | 4.9E-01 | 3.4E-01 | 3.5E-01 | 4.1E-01 | 4.1E-01 | 4.1E-01 | 4.1E-01 | 4.4E-01 | 4.4E-01 | 3.8E-01 | 3.8E-01 | 3.8E-01 | 3.8E-01 | 1.0E-02 | 4.1E-01 | 7.0E-01 | 3.0E-02 | 4.0E-01 | 4.2E-02 | 1.0 | 0.728 | 1.0 | 0.972 | 1.0 | 1.0 | 1.0 | 0.972 | 1.0 | 1.0 | 0.552 | 1.1 | 0.516 | |
| XC0312 | 5.6E-04 | 5.9E-04 | 6.5E-04 | 5.7E-04 | 6.8E-04 | 6.2E-04 | 5.7E-04 | 6.5E-04 | 6.9E-04 | 6.6E-04 | 6.0E-04 | 4.9E-05 | 6.3E-04 | 5.5E-05 | 5.5E-04 | 2.6E-05 | 6.6E-04 | 2.3E-05 | 1.0 | 0.860 | 0.9 | 0.222 | 1.1 | 0.140 | 1.1 | 0.140 | 1.1 | 0.370 | 1.2 | 0.005 | ** | | |
| XCD016 | 9.2E-04 | 7.4E-04 | 8.4E-04 | 6.4E-04 | 1.0E-03 | 8.5E-04 | 7.2E-04 | 6.7E-04 | 7.6E-04 | 1.1E-03 | 9.8E-04 | 8.8E-04 | 8.7E-05 | 8.7E-05 | 2.0E-04 | 7.2E-04 | 4.2E-05 | 9.7E-04 | 9.4E-05 | 1.0 | 0.804 | 0.9 | 0.128 | 1.2 | 0.135 | 1.1 | 0.482 | 1.4 | 0.027 | * | | | |
| XAD003 | 3.9E-04 | 4.4E-04 | 3.8E-04 | 7.7E-04 | 2.9E-04 | 4.4E-04 | 1.8E-04 | 3.9E-04 | 3.4E-04 | 3.9E-04 | 3.4E-04 | 3.9E-04 | 3.4E-04 | 3.9E-04 | 3.4E-04 | 3.9E-04 | 3.4E-04 | 3.9E-04 | 3.4E-04 | 1.0 | 0.950 | 0.8 | 0.427 | 1.5 | 0.216 | 1.7 | 0.350 | 1.7 | 0.437 | 1.7 | 0.157 | | |
| Gly-Asp | 2.1E-04 | 2.0E-04 | 2.5E-04 | 1.8E-04 | 2.8E-04 | 2.1E-04 | 2.0E-04 | 1.9E-04 | 2.3E-04 | 2.7E-04 | 2.3E-04 | 2.4E-04 | 2.2E-04 | 2.6E-05 | 2.2E-04 | 4.8E-05 | 2.1E-04 | 1.7E-05 | 2.5E-04 | 2.1E-05 | 1.0 | 0.859 | 1.0 | 0.594 | 1.1 | 0.219 | 1.1 | 0.525 | 1.2 | 0.072 | * | | |
| Thiamine | 8.1E-04 | 7.9E-04 | 8.8E-04 | 6.8E-04 | 8.6E-04 | 7.9E-04 | 1.0E-03 | 6.5E-04 | 5.4E-04 | 7.3E-04 | 9.8E-04 | 1.0E-03 | 8.3E-04 | 4.8E-05 | 8.5E-04 | 1.7E-04 | 6.4E-04 | 9.8E-05 | 4.1E-05 | 1.0 | 0.840 | 0.8 | 0.400 | 1.2 | 0.013 | ** | 1.2 | 0.283 | 1.5 | 0.013 | * | | |
| Thiamine phosphate | 3.3E-04 | 5.0E-04 | 3.7E-04 | 6.8E-04 | 2.9E-04 | 2.5E-04 | 4.2E-04 | 4.8E-04 | 4.2E-04 | 4.4E-04 | 3.3E-04 | 2.9E-04 | 4.0E-04 | 2.8E-05 | 4.1E-04 | 2.4E-04 | 4.4E-04 | 3.5E-05 | 3.5E-04 | 7.7E-05 | 1.0 | 0.964 | 1.1 | 0.548 | 0.9 | 0.515 | 0.9 | 0.733 | 0.8 | 0.181 | * | | |
| Xanthosine | 1.1E-03 | 8.1E-04 | 6.8E-04 | 6.3E-04 | 7.7E-04 | 1.1E-03 | 6.6E-04 | 7.3E-04 | 8.8E-04 | 7.5E-04 | 7.0E-04 | 8.3E-04 | 8.6E-04 | 2.5E-04 | 2.5E-04 | 3.7E-04 | 6.9E-05 | 7.8E-04 | 9.1E-05 | 1.0 | 0.958 | 0.9 | 0.579 | 0.9 | 0.779 | 0.9 | 0.722 | 0.9 | 0.173 | 1.1 | 0.492 | | |
| Citric acid | 4.9E-03 | 4.8E-03 | 4.1E-03 | 3.4E-03 | 5.7E-03 | 4.9E-03 | 4.9E-03 | 4.2E-03 | 4.2E-03 | 4.3E-03 | 3.6E-03 | 4.6E-03 | 4.6E-03 | 4.5E-04 | 4.7E-03 | 1.2E-03 | 4.4E-03 | 3.8E-04 | 4.2E-03 | 5.1E-04 | 1.0 | 0.938 | 1.0 | 0.642 | 0.9 | 0.317 | 0.9 | 0.536 | 0.9 | 0.493 | * | | |
| acetylneuraminat | 7.8E-02 | 6.5E-02 | 7.9E-02 | 7.6E-02 | 7.1E-02 | 7.4E-02 | 7.2E-02 | 7.7E-02 | 7.8E-02 | 8.4E-02 | 7.3E-02 | 7.8E-02 | 7.3E-02 | 7.5E-03 | 7.4E-02 | 2.5E-03 | 7.5E-02 | 3.4E-03 | 7.8E-02 | 5.5E-03 | 1.0 | 0.882 | 1.0 | 0.682 | 1.1 | 0.420 | 1.1 | 0.325 | ** | 1.0 | 0.514 | * | |
| His | 4.0E-04 | 4.0E-04 | 3.8E-04 | 3.9E-04 | 4.5E-04 | 3.9E-04 | 3.9E-04 | 4.2E-04 | 4.5E-04 | 4.7E-04 | 6.1E-04 | 6.5E-04 | 3.9E-04 | 7.6E-04 | 3.9E-04 | 7.6E-04 | 4.0E-04 | 5.1E-05 | 4.2E-04 | 3.1E-05 | 0.924 | 1.1 | 0.286 | 1.7 | 0.223 | ** | 1.7 | 0.009 | ** | 1.6 | 0.018 | | |
| Gly-Gly | 3.5E-02 | 2.2E-02 | 3.1E-02 | 3.4E-02 | 2.4E-02 | 2.9E-02 | 3.1E-02 | 3.4E-02 | 3.5E-02 | 1.2E-02 | 2.5E-02 | 2.0E-02 | 2.9E-02 | 6.6E-03 | 2.9E-02 | 4.7E-03 | 3.3E-02 | 2.2E-03 | 1.9E-02 | 6.6E-03 | 1.0 | 0.963 | 1.1 | 0.387 | 0.7 | 0.140 | 0.7 | 0.115 | 0.6 | 0.053 | * | | |
| Glucose 6-phosphate | 3.4E-03 | 2.0E-03 | 3.2E-03 | 3.8E-03 | 2.3E-03 | 2.4E-03 | 2.3E-03 | 2.7E-03 | 3.3E-03 | 3.1E-03 | 3.3E-03 | 3.1E-03 | 3.3E-03 | 2.9E-03 | 2.9E-03 | 2.5E-03 | 2.9E-03 | 3.0E-03 | 3.0E-03 | 2.9E-03 | 1.0 | 0.963 | 1.0 | 0.825 | 0.8 | 0.379 | 0.8 | 0.406 | 0.7 | 0.266 | * | | |
| AMP | 1.1E-01 | 1.1E-01 | 1.2E-01 | 9.7E-02 | 1.2E-01 | 1.2E-01 | 1.2E-01 | 1.2E-01 | 1.2E-01 | 1.7E-01 | 1.6E-01 | 1.6E-01 | 1.1E-01 | 2.5E-03 | 1.1E-01 | 1.3E-02 | 1.2E-01 | 3.0E-03 | 1.6E-01 | 6.4E-01 | 1.0 | 0.846 | 1.1 | 0.053 | 1.4 | 0.002 | ** | 1.4 | 0.010 | ** | 1.4 | 0.002 | ** |
| Creatinine | 1.3E-03 | 1.3E-03 | 9.9E-04 | 1.2E-03 | 1.4E-03 | 1.1E-03 | 1.1E-03 | 1.1E-03 | 1.1E-03 | 1.4E-03 | 1.0E-03 | 1.1E-03 | 1.2E-03 | 2.1E-04 | 1.2E-03 | 1.5E-04 | 1.1E-03 | 4.6E-05 | 2.2E-04 | 1.0 | 0.881 | 0.9 | 0.439 | 1.0 | 0.844 | 1.0 | 0.936 | 1.1 | 0.609 | 1.1 | 0.609 | 1.1 | 0.609 |
| Asn | 9.1E-03 | 6.3E-03 | 5.9E-03 | 7.4E-03 | 6.6E-03 | 6.9E-03 | 6.4E-03 | 6.3E-03 | 6.4E-03 | 7.5E-03 | 6.7E-03 | 6.7E-03 | 6.4E-03 | 9.0E-04 | 6.1E-03 | 4.0E-03 | 6.3E-03 | 3.7E-04 | 2.5E-04 | 1.1 | 0.834 | 0.9 | 0.976 | 1.0 | 0.976 | 0.9 | 0.650 | 0.9 | 0.285 | 0.9 | 0.439 | | |
| Kynurenine | 1.5E-04 | 1.6E-04 | 1.6E-04 | 2.1E-04 | 1.7E-04 | 8.5E-05 | 1.4E-04 | 1.2E-04 | 1.5E-04 | 1.7E-04 | 2.5E-04 | 2.6E-04 | 1.6E-04 | 9.1E-06 | 1.5E-04 | 6.2E-05 | 1.4E-04 | 1.1E-05 | 2.3E-04 | 4.7E-05 | 1.0 | 0.932 | 0.9 | 0.079 | 1.5 | 0.112 | 1.5 | 0.170 | 1.7 | 0.070 | 1.7 | 0.070 | |
| FD divalent | 1.2E-03 | 1.1E-03 | 1.2E-03 | 9.6E-04 | 1.2E-03 | 1.3E-03 | 1.1E-03 | 1.2E-03 | 1.3E-03 | 1.3E-03 | 1.1E-03 | 1.2E-03 | 1.3E-03 | 1.1E-03 | 1.2E-03 | 1.1E-03 | 1.4E-03 | 8.4E-05 | 1.1E-03 | 1.1E-04 | 1.0 | 0.800 | 0.9 | 0.305 | 1.1 | 0.412 | 1.1 | 0.464 | 1.1 | 0.181 | 1.1 | 0.181 | |
| N ² | 2.3E-04 | 1.3E-04 | 1.0E-04 | 1.4E-04 | 1.7E-04 | 1.4E-04 | 1.5E-04 | 1.4E-04 | 1.5E-04 | 1.7E-04 | 2.6E-04 | 1.6E-04 | 1.8E-04 | 1.5E-04 | 1.7E-04 | 3.0E-05 | 1.5E-04 | 1.5E-05 | 2.7E-05 | 2.0E-04 | 1.0 | 0.921 | 1.0 | 0.916 | 1.3 | 0.425 | 1.3 | 0.229 | 1.3 | 0.229 | 1.3 | 0.229 | |
| Acetylperindone | 2.5E-03 | 1.8E-03 | 2.4E-03 | 1.6E-03 | 2.3E-03 | 2.5E-03 | 1.5E-03 | 1.4E-03 | 1.8E-03 | 2.0E-03 | 1.6E-03 | 1.9E-03 | 2.2E-03 | 3.9E-04 | 2.1E-03 | 4.8E-04 | 1.6E-03 | 2.2E-04 | 1.8E-03 | 3.2E-04 | 1.0 | 0.851 | 0.7 | 0.069 | 0.8 | 0.232 | 0.9 | 0.425 | 1.2 | 0.188 | * | | |
| nic acid | 4.0E-02 | 3.8E-02 | 2.8E-02 | 3.1E-02 | 3.8E-02 | 3.5E-02 | 3.8E-02 | 3.6E-02 | 4.0E-02 | 4.2E-02 | 3.2E-02 | 3.4E-02 | 3.6E-02 | 5.7E-03 | 3.5E-02 | 3.6E-02 | 3.7E-02 | 2.3E-03 | 3.6E-02 | 5.1E-03 | 1.0 | 0.764 | 1.0 | 0.760 | 1.0 | 0.868 | 1.0 | 0.700 | 1.0 | 0.770 | 1.0 | 0.770 | |
| Pha | 1.6E-04 | 1.4E-04 | 1.6E-04 | 1.4E-04 | 1.7E-04 | 1.5E-04 | 1.7E-04 | 1.5E-04 | 1.7E-04 | 1.5E-04 | 1.7E-04 | 1.5E-04 | 1.7E-04 | 1.5E-04 | 1.7E-04 | 1.5E-04 | 1.7E-04 | 1.5E-04 | 1.7E-04 | 1.5E-04 | 1.0 | 0.807 | 1.0 | 0.680 | 0.9 | 0.183 | 0.9 | 0.536 | 0.9 | 0.100 | 0.9 | 0.100 | |
| Glycylneurami | 1.1E-03 | 1.1E-03 | 1.2E-03 | 9.0E-04 | 9.7E-04 | 1.4E-03 | 1.0E-03 | 1.1E-03 | 1.4E-03 | 1.3E-03 | 1.2E-03 | 1.2E-03 | 1.1E-03 | 5.0E-05 | 1.1E-03 | 3.2E-04 | 1.2E-03 | 1.8E-04 | 1.2E-03 | 4.2E-05 | 1.0 | 0.813 | 1.0 | 0.771 | 1.1 | 0.094 | 1.1 | 0.505 | 1.0 | 0.697 | 1.0 | 0.697 | |
| Threonic acid | 8.2E-04 | 6.4E-04 | 7.0E-04 | 6.1E-04 | 7.5E-04 | 7.1E-04 | 6.4E-04 | 6.8E-04 | 6.3E-04 | 6.9E-04 | 6.4E-04 | 6.4E-04 | 7.2E-04 | 9.1E-05 | 6.9E-04 | 7.1E-05 | 6.5E-04 | 2.6E-05 | 6.6E-04 | 3.0E-05 | 1.0 | 0.671 | 0.9 | 0.314 | 0.9 | 0.364 | 1.0 | 0.540 | 1.0 | 0.741 | 1.0 | 0.741 | |
| Ala-Ala | 7.2E-04 | 6.1E-04 | 7.2E-04 | 4.9E-04 | 7.3E-04 | 7.4E-04 | 7.2E-04 | 7.5E-04 | 6.1E-04 | 9.3E-04 | 6.8E-04 | 6.4E-04 | 9.3E-04 | 6.8E-04 | 6.4E-04 | 9.3E-04 | 6.8E-04 | 6.4E-04 | 9.3E-04 | 6.8E-04 | 1.1 | 0.741 | 1.1 | 0.180 | 1.4 | 0.012 | 1.4 | 0.069 | 1.2 | 0.010 | 1.2 | 0.010 | |
| Thiamine diphosphate | 5.2E-04 | 5.7E-04 | 5.3E-04 | 4.5E-04 | 5.6E-04 | 5.4E-04 | 4.4E-04 | 5.0E-04 | 4.9E-04 | 4.8E-04 | 3.8E-04 | 3.8E-04 | 5.4E-04 | 2.7E-05 | 5.1E-04 | 6.0E-05 | 4.8E-04 | 3.1E-05 | 4.1E-04 | 6.1E-05 | 0.9 | 0.514 | 0.9 | 0.057 | 0.8 | 0.046 | ** | 0.8 | 0.098 | 0.9 | 0.172 | 0.9 | 0.172 |
| Dithiothalamate | 2.0E-04 | 1.7E-04 | 2.8E-04 | 3.0E-04 | 1.7E-04 | 1.4E-04 | 3.1E-04 | 1.1E-04 | 1.4E-04 | 1.4E-04 | 1.4E-04 | 1.4E-04 | 1.4E-04 | 2.1E-04 | 5.7E-05 | 2.0E-04 | 8.5E-05 | 1.8E-04 | 1.1E-04 | 4.8E-04 | 0.9 | 0.851 | 0.9 | 0.704 | 0.8 | 0.439 | 0.9 | 0.695 | 1.0 | 0.932 | 1.0 | 0.932 | |
| NAD ⁺ | 1.6E-02 | 2.5E-02 | 2.5E-02 | 1.5E-02 | 2.3E-02 | 2.4E-02 | 2.0E-02 | 2.1E-02 | 2.3E-02 | 1.6E-02 | 1.6E-02 | 1.6E-02 | 2.2E-02 | 5.3E-03 | 2.1E-02 | 6.3E-03 | 2.1E-02 | 1.3E-03 | 1.6E-02 | 5.6E-04 | 0.9 | 0.786 | 1.0 | 0.854 | 0.7 | 0.172 | 0.8 | 0.237 | 0.7 | 0.009 | ** | | |
| XC0137 | 5.8E-03 | 5.8E-03 | 5.3E-03 | 5.3E-03 | 5.3E-03 | 5.3E-03 | 5.3E-03 | 5.3E-03 | 5.3E-03 | 5.3E-03 | 5.3E-03 | 5.3E-03 | 5.3E-03 | 5.3E-03 | 5.3E-03 | 5.3E-03 | 5.3E-03 | 5.3E-03 | 5.3E-03 | 5.3E-03 | 1.1 | 0.834 | 0.9 | 0.650 | 0.9 | 0.285 | 0.9 | 0.439 | 0.9 | | | | |

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------------------------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|------|-------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|----|--|
| Butyrylcamitine | 8.7E-03 | 3.4E-03 | 6.9E-03 | 8.6E-04 | 4.4E-03 | 3.2E-03 | 2.0E-02 | 2.7E-02 | 2.1E-02 | 7.1E-03 | 8.6E-03 | 5.9E-03 | 6.3E-03 | 2.7E-03 | 2.8E-03 | 1.8E-03 | 2.3E-02 | 3.6E-03 | 7.2E-03 | 1.3E-03 | 0.4 | 0.140 | 3.6 | 0.004 | ** | 1.1 | 0.645 | 2.6 | 0.030 | * | 0.3 | 0.010 | ** | |
| 5-Aminovaleric acid | 1.2E-02 | 1.1E-02 | 1.4E-02 | 3.8E-03 | 7.6E-03 | 4.6E-03 | 1.2E-02 | 1.1E-02 | 1.3E-02 | 8.3E-03 | 8.9E-03 | 8.6E-03 | 1.2E-02 | 1.6E-03 | 5.4E-03 | 2.0E-03 | 1.2E-02 | 6.8E-04 | 8.6E-03 | 2.9E-04 | 0.4 | 0.011 | * | 1.0 | 0.696 | 0.7 | 0.054 | 1.6 | 0.104 | 0.7 | 0.007 | ** | | |
| 2-Aminoadipic acid | 6.2E-03 | 2.6E-03 | 1.6E-03 | 1.2E-03 | 1.5E-03 | 1.5E-03 | 2.3E-03 | 2.1E-03 | 1.7E-03 | 3.0E-03 | 2.3E-03 | 1.8E-03 | 3.5E-03 | 2.4E-03 | 1.4E-03 | 1.7E-04 | 2.1E-03 | 3.2E-04 | 2.4E-03 | 5.9E-04 | 0.4 | 0.275 | 0.6 | 0.417 | 0.7 | 0.516 | 1.7 | 0.097 | 1.2 | 0.479 | | | | |
| XX0040 | 6.1E-04 | 7.4E-04 | 8.0E-04 | 1.6E-04 | 4.2E-04 | 2.2E-04 | 7.4E-04 | 7.3E-04 | 5.6E-04 | 4.8E-04 | 5.4E-04 | 6.8E-04 | 7.2E-04 | 9.7E-05 | 2.7E-04 | 1.3E-04 | 6.7E-04 | 9.9E-05 | 5.7E-04 | 1.0E-04 | 0.4 | 0.011 | * | 0.9 | 0.601 | 0.8 | 0.138 | 2.1 | 0.039 | * | 0.8 | 0.268 | | |
| N ⁵ -Methyllysine | 5.9E-04 | 3.9E-04 | 3.9E-04 | 1.9E-04 | 1.7E-04 | 1.3E-04 | 5.1E-04 | 4.7E-04 | 4.9E-04 | 2.0E-04 | 2.9E-04 | 2.3E-04 | 4.6E-04 | 1.1E-04 | 1.6E-04 | 2.7E-05 | 4.9E-04 | 2.3E-05 | 2.4E-04 | 4.7E-05 | 0.4 | 0.039 | * | 1.1 | 0.657 | 0.5 | 0.063 | 1.5 | 0.085 | 0.5 | 0.004 | ** | | |
| 1H-Imidazole-4-propionic acid | 3.0E-04 | 1.9E-04 | 3.5E-04 | 7.0E-05 | 1.5E-04 | 6.7E-05 | 4.3E-04 | 2.0E-04 | 2.4E-04 | 9.1E-05 | 9.3E-05 | 8.3E-05 | 2.8E-04 | 8.1E-05 | 9.7E-05 | 4.9E-05 | 2.9E-04 | 1.2E-04 | 8.9E-05 | 5.0E-06 | 0.3 | 0.036 | * | 1.0 | 0.933 | 0.3 | 0.053 | 0.9 | 0.804 | 0.3 | 0.102 | | | |
| Betonicine | 5.5E-04 | 4.7E-04 | 6.7E-04 | 1.3E-04 | 2.8E-04 | 1.6E-04 | 5.7E-04 | 6.1E-04 | 5.1E-04 | 3.8E-04 | 5.6E-04 | 4.2E-04 | 5.6E-04 | 9.7E-05 | 1.9E-04 | 7.6E-05 | 5.6E-04 | 5.5E-05 | 4.5E-04 | 9.4E-05 | 0.3 | 0.007 | ** | 1.0 | 0.393 | 0.8 | 0.234 | 2.4 | 0.021 | * | 0.8 | 0.176 | | |
| Ethyl | 1.7E-03 | 8.3E-04 | 2.8E-03 | 7.9E-04 | 4.8E-04 | 2.0E-04 | 5.4E-04 | 1.5E-03 | 1.4E-03 | 1.3E-03 | 4.9E-03 | 3.2E-03 | 1.9E-03 | 1.0E-03 | 4.9E-04 | 3.0E-04 | 1.2E-03 | 5.4E-04 | 3.1E-03 | 1.9E-03 | 0.3 | 0.149 | 0.7 | 0.420 | 1.8 | 0.337 | 6.3 | 0.122 | 2.7 | 0.192 | | | | |
| UDP-glucuronic acid | 4.6E-03 | 4.4E-03 | 5.9E-03 | 3.5E-04 | 2.0E-03 | 6.6E-04 | 4.3E-03 | 3.7E-03 | 2.7E-03 | 1.8E-03 | 3.2E-03 | 3.5E-03 | 5.0E-03 | 7.7E-04 | 1.0E-03 | 8.6E-04 | 3.6E-03 | 8.1E-04 | 2.8E-03 | 8.9E-04 | 0.2 | 0.004 | ** | 0.7 | 0.092 | 0.6 | 0.034 | * | 2.8 | 0.064 | 0.8 | 0.343 | | |
| Putrescine | 1.6E-03 | 1.6E-03 | 2.3E-03 | 1.7E-04 | 1.9E-04 | 1.0E-04 | 1.4E-03 | 1.4E-03 | 8.8E-04 | 1.5E-04 | 6.2E-04 | 3.3E-04 | 1.8E-03 | 3.8E-04 | 1.5E-04 | 4.6E-05 | 1.2E-03 | 3.1E-04 | 3.7E-04 | 2.3E-04 | 0.09 | 0.016 | * | 0.7 | 0.111 | 0.2 | 0.009 | ** | 2.4 | 0.251 | 0.3 | 0.021 | * | |
| N-Methylalanine | 2.3E-04 | 1.6E-04 | 1.4E-04 | N.D. | N.D. | N.D. | N.D. | 1.1E-04 | N.D. | 1.4E-04 | 1.4E-04 | N.D. | 1.8E-04 | 4.5E-05 | N.D. | N.A. | 1.1E-04 | N.A. | 1.4E-04 | 1.4E-06 | <1 | N.A. | 0.6 | N.A. | 0.8 | 0.324 | <1 | N.A. | 1.3 | N.A. | N.A. | | | |
| Butyric acid | N.D. | N.D. | N.D. | N.D. | N.D. | N.D. | 3.1E-04 | 6.4E-04 | 3.5E-04 | N.D. | 2.9E-04 | N.D. | N.D. | N.A. | N.D. | N.A. | 4.4E-04 | 1.8E-04 | 2.9E-04 | N.A. | N.A. | 1< | N.A. | 1< | N.A. | 1< | N.A. | 1< | N.A. | 0.7 | N.A. | N.A. | | |
| Cytosine | N.D. | N.D. | N.D. | N.D. | N.D. | N.D. | 4.3E-05 | 5.7E-05 | 8.7E-05 | N.D. | N.D. | N.D. | N.D. | N.A. | N.D. | N.A. | 6.2E-05 | 2.2E-05 | N.D. | N.A. | N.A. | 1< | N.A. | 1< | N.A. | N.A. | N.A. | N.A. | N.A. | <1 | N.A. | N.A. | | |

N.D.: Not Detected.

N.A.: Not Available.

† in the case of A vs B, the ratio of the average was calculated as A/B.

‡ Welch's t-test, p-value (*<0.05, **<0.01, ***<0.001)

Description of XA... or XC... in compound name indicates unknown peaks, which has been detected in some other organism samples in the HMT database for metabolite identification.