

Table S6. Level of metabolite identification for metabolites detected on LC/MS with authenticated standards

| Metabolite | Retention time | Accurate mass | Obtained mass | ppm error | Level of identification |
|-------------------------|----------------|---------------|---------------|-----------|-------------------------|
| Cholesteryl sulfate | 1.109 | 465.3034 | 465.30439 | 2.13 | 2 |
| Myristic acid | 1.225 | 227.2015 | 227.2015133 | 0.06 | 1 |
| 4-Pyridoxic acid | 1.457 | 182.0458 | 182.0748878 | 159.78 | 2 |
| Uracil | 2.769 | 111.0198 | 111.0198336 | 0.30 | 1 |
| Adenine | 3.647 | 134.0466 | 134.0471054 | 3.77 | 1 |
| Biotin | 4.4 | 243.0801 | 243.0628296 | -71.05 | 2 |
| Deoxycytidine | 5.039 | 226.0827 | 226.0830372 | 1.49 | 1 |
| Phenylalanine | 5.136 | 164.0713 | 164.0711262 | -1.06 | 1 |
| Pyroglutamic acid | 5.17 | 128.0354 | 128.0354362 | 0.28 | 1 |
| D-Galactono-1,4-lactone | 5.401 | 177.0401 | 177.0408104 | 4.01 | 1 |
| D-Glucosamine | 5.57 | 178.0715 | 178.0373009 | -192.05 | 2 |
| Leucine | 5.965 | 130.0872 | 130.0871399 | -0.46 | 1 |
| Cytidine | 6.084 | 242.0774 | 242.0893372 | 49.31 | 2 |
| L-Tryptophan | 6.214 | 203.082 | 203.0784241 | -17.61 | 2 |
| Uridine | 6.28 | 243.0614 | 243.0605659 | -3.43 | 1 |
| Tryptophan | 6.5 | 203.0824 | 203.0784241 | -19.58 | 1 |
| Betaine | 6.68 | 116.0716 | 116.9164906 | 7279.05 | 2 |
| L-Valine | 6.695 | 116.0717 | 116.9164906 | 7278.18 | 2 |
| Guanosine | 6.72 | 282.0844 | 282.0780182 | -22.62 | 2 |
| Proline | 6.796 | 114.0555 | 114.0558809 | 3.34 | 1 |
| Uric Acid | 6.927 | 167.0208 | 167.0390625 | 109.34 | 2 |
| Tyrosine | 7.3 | 180.0664 | 180.0664001 | 0.00 | 1 |
| 2-Oxobutanoate | 7.374 | 101.0242 | 101.0415018 | 171.26 | 2 |
| Mannitol | 7.492 | 181.0709 | 181.1877888 | 645.54 | 2 |
| Lactate | 7.6 | 89.0245 | | | 2 |

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|-----------------------|-------|----------|-------------|--------|---|
| D-fructose | 7.953 | 179.0557 | 179.0557507 | 0.28 | 1 |
| Glycine | 8.03 | 74.0254 | | | 2 |
| Alanine | 8.182 | 88.0409 | | | 2 |
| Histidine | 8.238 | 154.0619 | 154.0619934 | 0.61 | 1 |
| sn-Glycerol-3P | 8.371 | 171.0059 | 171.0406616 | 203.28 | 2 |
| dUMP | 8.388 | 307.0331 | 307.0340622 | 3.13 | 1 |
| AMP | 8.503 | 346.0558 | 346.0559738 | 0.50 | 1 |
| Glutathione | 8.588 | 306.0758 | 306.0595459 | -53.10 | 2 |
| Asparagine | 8.609 | 131.0463 | 131.0460869 | -1.63 | 2 |
| Glutamic acid | 8.653 | 146.0456 | 146.0419224 | -25.18 | 2 |
| NADH | 8.742 | 662.1009 | 662.1015106 | 0.92 | 1 |
| Aspartic acid | 8.808 | 132.0299 | 132.0303326 | 3.28 | 1 |
| 2-Deoxy-D-ribose-5P | 8.808 | 213.0165 | 213.0167023 | 0.95 | 1 |
| Cellobiose | 8.818 | 341.1069 | 341.1089493 | 6.01 | 1 |
| D-Galacturonate | 9 | 193.035 | 193.0279968 | -36.28 | 2 |
| Citrulline | 9.048 | 174.0875 | 174.1066437 | 109.97 | 2 |
| Ornithine | 9.067 | 131.0824 | 131.0824055 | 0.04 | 1 |
| dCMP | 9.101 | 306.0483 | 306.048793 | 1.61 | 1 |
| UMP | 9.166 | 323.0285 | 323.0286774 | 0.55 | 1 |
| DL-Glyceraldehyde-3P | 9.233 | 168.9909 | 168.990797 | -0.61 | 1 |
| GMP | 9.3 | 362.0513 | 362.0517848 | 1.34 | 1 |
| CMP | 9.3 | 322.0436 | 322.0446846 | 3.37 | 1 |
| 2-Dehydro-D-gluconate | 9.313 | 193.0344 | 193.0279968 | -33.17 | 2 |
| ADP | 9.382 | 426.021 | 426.0226723 | 3.93 | 1 |
| Fumarate | 9.415 | 115.0033 | 115.0089157 | 48.83 | 2 |
| Malate (Malic acid) | 9.465 | 133.0138 | 133.0142193 | 3.15 | 1 |
| D-Ribose-5P | 9.5 | 229.0113 | 229.0123837 | 4.73 | 1 |
| Malate | 9.512 | 133.0138 | 133.0142193 | 3.15 | 1 |

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|---------------------------|--------|----------|-------------|----------|---|
| UDP-D-Glucose | 9.852 | 565.0471 | 565.0475337 | 0.77 | 1 |
| O-phospho-L-serine | 9.946 | 184.0011 | 184.0011215 | 0.12 | 1 |
| D-Glucosamine-1P | 9.968 | 258.0388 | 258.0381012 | -2.71 | 1 |
| ATP | 9.97 | 505.9888 | 505.9889832 | 0.36 | 1 |
| D-Glucose-6P | 10.1 | 259.022 | 259.0222031 | 0.78 | 1 |
| IDP | 10.151 | 427.007 | 427.0075508 | 1.29 | 1 |
| Phosphoenolpyruvate | 10.526 | 166.9749 | 166.973777 | -6.73 | 1 |
| Isoleucine | 10.758 | 191.0191 | | | 2 |
| Isocitrate | 10.758 | 191.0191 | | | 2 |
| Citrate | 10.772 | 191.0197 | | | 2 |
| CTP | 11.013 | 481.9758 | 481.126783 | -1761.53 | 2 |
| Fructose 1/6-bisphosphate | 11.046 | 338.9877 | 338.994133 | 18.98 | 2 |
| Lysine | 12.862 | 145.0984 | 145.0982189 | -1.25 | 1 |
| Arginine | 13.177 | 173.1042 | 173.1042419 | 0.24 | 1 |

A metabolite with ppm error $\leq \pm 10$ is considered a level 1 identified metabolites.

A metabolite with ppm error $> \pm 10$ is characterised as a level 2 putative compound.