

**Supplementary Table 1.** Limit of detection for measured analytes

| Analyte                        | LOD (μM) |
|--------------------------------|----------|
| Creatinine                     | 6.34     |
| Glycine                        | 0.97     |
| Alanine                        | 0.55     |
| Serine                         | 0.307    |
| Histamine                      | 0.00698  |
| Proline                        | 0.0945   |
| Valine                         | 0.205    |
| Threonine                      | 0.556    |
| Taurine                        | 0.611    |
| Putrescine                     | 0.0625   |
| 4-Hydroxyproline               | 0.0857   |
| Leucine                        | 0.789    |
| Isoleucine                     | 0.306    |
| Asparagine                     | 0.472    |
| Aspartic acid                  | 2.73     |
| Glutamine                      | 0.422    |
| Glutamic acid                  | 0.967    |
| Methionine                     | 0.191    |
| Dopamine                       | 0.0109   |
| Histidine                      | 0.142    |
| α-Aminoadipic acid             | 0.735    |
| Phenylalanine                  | 0.0671   |
| Methionine sulfoxide           | 0.268    |
| Arginine                       | 0.0318   |
| N <sup>2</sup> -Acetylorithine | 0.0647   |
| Serotonin                      | 0.0164   |
| Tyrosine                       | 0.0818   |
| DOPA                           | 0.00674  |
| Asymmetric dimethylarginine    | 0.0169   |
| Symmetric dimethylarginine     | 0.0139   |
| Tryptophan                     | 0.0470   |
| Kynurenine                     | 0.0286   |
| Carnosine                      | 0.0362   |
| Ornithine                      | 0.0439   |

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| Lysine                              | 0.131  |
| Spermidine                          | 0.0125 |
| Spermine                            | 0.0103 |
| Sarcosine                           | 0.143  |
| N1,N12-Diacetylspermine             | 0.0128 |
| Tyramine                            | 0.0371 |
| Creatine                            | 0.198  |
| Betaine                             | 0.701  |
| Choline                             | 1.33   |
| Trimethylamine N-oxide              | 0.631  |
| 1-Methylhistidine/3-Methylhistidine | 0.0840 |
| Lactic acid                         | 1.04   |
| 3-Hydroxybutyric acid               | 0.205  |
| alpha-Ketoglutaric acid             | 0.258  |
| Citric acid                         | 2.58   |
| Butyric acid                        | 0.133  |
| HPHPA                               | 0.0495 |
| p-Hydroxyhippuric acid              | 0.269  |
| Succinic acid                       | 0.121  |
| Fumaric acid                        | 0.0135 |
| Pyruvic acid                        | 0.0628 |
| Isobutyric acid                     | 0.0832 |
| Hippuric acid                       | 0.493  |
| Methylmalonic acid                  | 0.0309 |
| Homovanillic acid                   | 0.393  |
| Indoleacetic acid                   | 0.852  |
| Uric acid                           | 1.37   |
| Glucose                             | 8.37   |
| LysoPC a C14:0                      | 1.25   |
| LysoPC a C16:1                      | 0.124  |
| LysoPC a C16:0                      | 0.235  |
| LysoPC a C17:0                      | 0.115  |
| LysoPC a C18:2                      | 0.241  |
| LysoPC a C18:1                      | 0.107  |
| LysoPC a C18:0                      | 0.149  |
| LysoPC a C20:4                      | 0.176  |

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| LysoPC a C20:3                      | 0.143  |
| LysoPC a C24:0                      | 0.422  |
| LysoPC a C26:1                      | 0.0922 |
| LysoPC a C26:0                      | 0.105  |
| LysoPC a C28:1                      | 0.0519 |
| LysoPC a C28:0                      | 0.349  |
| SM(OH) C14:1                        | 0.119  |
| SM C16:1                            | 0.0211 |
| SM C16:0                            | 0.0396 |
| SM(OH) C16:1                        | 0.0128 |
| SM C18:1                            | 0.0171 |
| PC aa C32:2                         | 0.0847 |
| SM C18:0                            | 0.0361 |
| SM C20:2                            | 0.203  |
| PC ae C36:0                         | 0.0379 |
| PC aa C36:6                         | 0.0348 |
| PC aa C36:0                         | 0.068  |
| SM(OH) C22:2                        | 0.0279 |
| SM(OH) C22:1                        | 0.0268 |
| PC aa C38:6                         | 0.0164 |
| PC aa C38:0                         | 0.677  |
| PC ae C40:6                         | 0.101  |
| SM(OH) C24:1                        | 0.0291 |
| PC aa C40:6                         | 0.0974 |
| PC aa C40:2                         | 0.0125 |
| PC aa C40:1                         | 0.299  |
| Carnitine (C0)                      | 4.24   |
| L-Acetylcarnitine (C2)              | 0.602  |
| Propenoylcarnitine (C3:1)           | 0.101  |
| Propionylcarnitine (C3)             | 0.0853 |
| Butenylcarnitine (C4:1)             | 0.0419 |
| Butyrylcarnitine (C4)               | 0.108  |
| Hydroxypropionylcarnitine<br>(C3OH) | 0.0387 |
| Tiglylcarnitine (C5:1)              | 0.0463 |
| Valerylcarnitine (C5)               | 0.0549 |
| Hydroxybutyrylcarnitine (C4OH)      | 0.0404 |

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| Hexenoylcarnitine (C6:1)                     | 0.0552 |
| Hexanoylcarnitine (C6)                       | 0.127  |
| Hydroxyvalerylcarnitine (C5OH)               | 0.0397 |
| Glutaconylcarnitine (C5:1DC)                 | 0.0302 |
| Glutaryl carnitine (C5DC)                    | 0.0206 |
| Octanoylcarnitine (C8)                       | 0.206  |
| Methylglutaryl carnitine (C5MDC)             | 0.0312 |
| Nonaylcarnitine (C9)                         | 0.0225 |
| Pimelylcarnitine (C7DC)                      | 0.0208 |
| Decadienylcarnitine (C10:2)                  | 0.0171 |
| Decenoylcarnitine (C10:1)                    | 0.127  |
| Decanoylcarnitine (C10)                      | 0.0382 |
| Dodecenoylcarnitine (C12:1)                  | 0.0644 |
| Dodecanoylcarnitine (C12)                    | 0.0218 |
| Tetradecadienylcarnitine (C14:2)             | 0.0113 |
| Tetradecenoylcarnitine (C14:1)               | 0.0689 |
| Tetradecanoylcarnitine (C14)                 | 0.0724 |
| Dodecanedioylcarnitine (C12DC)               | 0.0877 |
| Hydroxytetradecadienylcarnitine<br>(C14:2OH) | 0.0789 |
| Hydroxytetradecenoylcarnitine<br>(C14:1OH)   | 0.0927 |
| Hexadecadienylcarnitine (C16:2)              | 0.0239 |
| Hexadecenoylcarnitine (C16:1)                | 0.0384 |
| Hexadecanoylcarnitine (C16)                  | 0.0117 |
| Hydroxyhexadecadienylcarnitine<br>(C16:2OH)  | 0.0654 |
| Hydroxyhexadecenoylcarnitine<br>(C16:1OH)    | 0.0119 |
| Hydroxyhexadecanoylcarnitine<br>(C16OH)      | 0.0799 |
| Octadecadienylcarnitine (C18:2)              | 0.0954 |
| Octadecenoylcarnitine (C18:1)                | 0.0899 |
| Octadecanoylcarnitine (C18)                  | 0.0676 |
| Hydroxyoctadecenoylcarnitine<br>(C18:1OH)    | 0.0658 |