**Table S1** Detailed information of the identified primary metabolites

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Number | Compound name | Library similarity (%) | Retention index | Retention time |
| **Amino acids** |
| 6 | GlycylglycineSerineL-NorleucineL-ThreonineL-HomoserineL-ProlineL-AlanineGlutamineL-AsparagineGlycineL-ValineL-Aspartic acid | 75 | 1669 | 6.864 |
| 7 | 78 | 1158 | 7.476 |
| 8 | 71 | 1336 | 7.924 |
| 11 | 90 | 1193 | 8.551 |
| 15 | 74 | 1421 | 11.651 |
| 18 | 94 | 1466 | 15.956 |
| 23 | 87 | 1038 | 19.615 |
| 24 | 83 | 1612 | 19.807 |
| 25 | 91 | 1745 | 21.627 |
| 35 | 84 | 1061 | 29.317 |
| 36 | 80 | 1172 | 29.565 |
| 45 | 75 | 1512 | 35.503 |
| **Organic acid** |
| 1 | Propanoic acidEthanedioic acidAcetic acidMalic acidButanoic acid2-Keto-d-gluconic acidAcetoxyacetic acid3,4-Dimethoxymandelic acid3,5-Dimethoxymandelic acid2,5-Dimethoxymandelic acidHexadecanoic acid9,12-Octadecadienoic acid | 92 | 915 | 3.576 |
| 3 | 97 | 971 | 4.66 |
| 10 | 80 | 880 | 8.094 |
| 17 | 93 | 1390 | 15.213 |
| 19 | 72 | 1260 | 16.324 |
| 31 | 85 | 2073 | 26.851 |
| 38 | 76 | 1977 | 29.919 |
| 39 | 78 | 1867 | 31.885 |
| 40 | 78 | 1867 | 32.494 |
| 42 | 83 | 1867 | 34.054 |
| 43 | 91 | 1987 | 34.375 |
| 53 | 79 | 2202 | 43.233 |
| 54 | Oleic acid | 83 | 2194 | 43.595 |
| 55 | Heptadecanoic acid | 80 | 2087 | 45.196 |
| 61 | Octadecanoic acid | 93 | 2780 | 63.83 |
| 63 | Cholan-24-oic acid | 74 | 2922 | 75.537 |
| **Sugars** |
| 14 | MannoseD-Erythro-PentopyranoseSorbopyranoseD-FructoseGlucopyranoseD-Glucoseβ-D-Galactopyranosideα-D-Glucopyranoside | 77 | 1686 | 10.731 |
| 21 | 75 | 1446 | 18.156 |
| 32 | 84 | 2049 | 27.161 |
| 34 | 88 | 1982 | 28.218 |
| 37 | 95 | 2037 | 29.717 |
| 41 | 96 | 1970 | 33.618 |
| 51 | 74 | 1991 | 40.395 |
| 60 | 94 | 3552 | 61.605 |
| **Alcohol** |
| 16 | 2,3-ButanediolInositolStigmasterolβ-Sitosterol9,19-Cyclolanostan-3-ol | 76 | 941 | 12.57 |
| 49 | 84 | 2194 | 38.196 |
| 62 | 91 | 2797 | 74.784 |
| 64 | 83 | 2789 | 76.335 |
| 65 | 83 | 2834 | 76.834 |
| **Others** |
| 5 | AcetamideN-Methyl-2-(2-hydroxyphenyl)ethylamine3,5-Dimethoxymandelic amide1H-Indole-3-ethanamine4-Imidazolidinone2-PyrrolidinethioneBenzeneethanamineEthylenediamine1,4-ButanediamineCadaverine3,4-Dimethoxyphenylacetone | 74 | 563 | 6.341 |
| 22 | 87 | 1548 | 18.911 |
| 26 | 78 | 1734 | 22.738 |
| 28 | 86 | 1839 | 24.522 |
| 33 | 80 | 1683 | 27.687 |
| 46 | 70 | 1613 | 36.357 |
| 47 | 86 | 2174 | 36.583 |
| 48 | 79 | 1557 | 37.773 |
| 52 | 82 | 1350 | 41.68 |
| 56 | 83 | 1449 | 54.685 |
| 59 | 79 | 1507 | 60.32 |
| **Impurities** |  |  |  |  |
| 4 | Pentasiloxane | 96 | 0 | 4.448 |
| 9 | Silanol | 94 | 1068 | 5.56 |
| 12 | Trisiloxane | 93 | 0 | 8.034 |
| 13 | Asparagine | 85 | 698 | 9.456 |
| 20 | Silane | 70 | 1754 | 10.496 |
| 29 | Phenylpropanolamine | 91 | 1498 | 17.467 |
| 30 | 1-Methyl-5-mercaptotetrazole | 90 | 1555 | 25.771 |
| 44 | Silanamine | 83 | 0 | 26.49 |
| 50 | Tyrosine | 78 | 1394 | 34.876 |
| 57 | 1,3-Dipalmitin | 63 | 2087 | 39.067 |
| 58 | Dimethyl-(isopropyl)-silyloxybenzene | 76 | 4055 | 58.067 |
| **Internal standard** |  |  |  |  |
| 27 | Ribitol | 88 | 1746 | 24.258 |