**Table S3** Identification of related marker metabolites of Jigucao capsule based on urine metabolic spectrum

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **NO.** | **Rt** | **Metabolite** | **Molecular** | **Ion** | **m/z** | **Error** | **T’TEST** | **Trend** | **JGCC** |
| **Name** | **Formula** | **form** | **determined** | （mDa） |
| 1 | 0.82 | *Cis*-Aconitic acid | C6H6O6 | [M-H]- | 173.0084 | -0.2 | 0.007790 | ↑ | - |
| 2 | 1.02 | 2,3-Dihydroxyvaleric acid | C5H10O4 | [2M-H]- | 267.1098 | 1.8 | 0.039910 | ↑ | √ |
| 3 | 1.51 | 2-Methoxyestrone | C19H24O3 | [M-H]- | 299.1665 | -4.5 | 0.027107 | ↑ | √ |
| 4 | 1.58 | Urocanic acid | C6H6N2O2 | [M+H]+ | 139.0509 | 0.5 | 0.013914 | ↓ | √## |
| 5 | 1.78 | Malonylcarnitine | C10H17NO6 | [M+FA-H]- | 292.1054 | 2.2 | 0.037834 | ↓ | - |
| 6 | 2.06 | N-(1-Deoxy-1-fructosyl)methionine | C11H21NO7S | [M+H]+ | 312.1089 | 1.6 | 0.046442 | ↑ | √ |
| 7 | 3.15 | Phenylpyruvic acid | C9H8O3 | [M+H]+ | 165.0559 | 0.7 | 0.004537 | ↑ | - |
| 8 | 3.18 | Glucosamine | C6H13NO5 | [M+H]+ | 180.0883 | 1.1 | 0.040401 | ↑ | √# |
| 9 | 3.95 | Adrenochrome | C9H9NO3 | [M+FA-H]- | 224.0560 | 0.1 | 0.000361 | ↑ | √## |
| 10 | 5.16 | 5-Hydroxy-6-methoxyindole glucuronide | C15H17NO8 | [M-H]- | 338.0888 | 0.7 | 0.021314 | ↓ | - |
| 11 | 5.22 | 5-Methoxyindoleacetate | C11H11NO3 | [M+FA-H]- | 250.0717 | 0.2 | 0.000002 | ↑ | √ |
| 12 | 5.93 | 1H-Indole-3-carboxaldehyde | C9H7NO | [M+H]+ | 146.0607 | 2.3 | 0.003512 | ↓ | √ |
| 13 | 6.04 | Dodecanoic acid | C12H24O2 | [M+FA-H]- | 245.1749 | -0.6 | 0.023037 | ↑ | √# |
| 14 | 6.73 | Pyridoxal | C8H9NO3 | [2M-H]- | 333.1129 | -3.5 | 0.007254 | ↑ | √# |
| 15 | 7.19 | Tryptophanol | C10H11NO | [2M-H]- | 321.1579 | -2.4 | 0.001160 | ↑ | √## |
| 16 | 7.37 | Homocarnosine | C10H16N4O3 | [M+Na]+ | 263.1119 | 0.9 | 0.009323 | ↑ | - |
| 17 | 7.43 | *Trans*-Dodec-2-enoic acid | C12H22O2 | [M+FA-H]- | 243.1600 | 0.4 | 0.016868 | ↑ | √# |
| 18 | 7.47 | Mesobilirubinogen | C33H44N4O6 | [M+H]+ | 593.3384 | 4.5 | 0.006352 | ↓ | √ |
| 19 | 7.49 | 3-Hydroxydodecanedioic acid | C12H22O5 | [M-H]- | 245.1383 | -0.6 | 0.014050 | ↑ | √ |
| 20 | 7.80 | Kynurenic acid | C10H7NO3 | [2M-H]- | 377.0771 | -0.3 | 0.037443 | ↑ | √ |
| 21 | 8.09 | *L*-Urobilin | C33H46N4O6 | [M+H]+ | 595.3488 | -0.8 | 0.024033 | ↑ | √# |
| 22 | 8.66 | Arachidonic acid | C20H32O2 | [M+Na]+ | 327.2318 | 4.6 | 0.039426 | ↑ | √# |
| 23 | 8.99 | 7-Ketodeoxycholic acid | C24H38O5 | [M+H]+ | 407.2786 | -1.1 | 0.014785 | ↑ | - |
| 24 | 9.02 | 3-Sulfodeoxycholic acid | C23H38O7S | [M+FA-H]- | 503.2353 | 4.0 | 0.005663 | ↑ | √ |
| 25 | 9.17 | 7a,12a-Dihydroxy-3-oxo-4-cholenoic acid | C24H36O5 | [M+H]+ | 405.2635 | 1.0 | 0.044066 | ↑ | √ |
| ↓：Decreased,↑：Increased, Model vs Control. -: Compared with the model, JGCC group was no tendency to approach the control group; √: Compared with the model, JGCC group showed a tendency to approach the control group; (#P<0.05; ##P<0.01). | | | | | | | | | |