**Table S2** Secondary fragmentation of potential biomarkers in the urine of dampness-heat jaundice model rats

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **NO** | **Rt** | **m/z determined** | **Proposed Composition** | **Postulated Identity** | **MS/MS** | **Structural Formula** |
| 1 | 0.82 | 173.0084 | C6H6O6 | *Cis*-Aconitic acid | 173.0458[M-H]-, 129.0578[M-H-CO2]-, 111.0492[M-H-CH2O3]-, 85.0714[M-H-C2O4]- |  |
| 2 | 1.02 | 267.1098 | C5H10O4 | 2,3-Dihydroxyvaleric acid | 267.1389[2M-H]-, 187.1087[2M-H-CH4O4]- |  |
| 3 | 1.51 | 299.1665 | C19H24O3 | 2-Methoxyestrone | 299.1602[M-H]-, 251.1118[M-H-C2H8O]- |  |
| 4 | 1.58 | 139.0509 | C6H6N2O2 | Urocanic acid | 139.0513[M+H]+,122.0280[M+H-NH3]+, 96.0481[M+H-C2H5N]+ |  |
| 5 | 1.78 | 292.1054 | C10H17NO6 | Malonylcarnitine | 292.1316[M+FA-H]-, 188.0419[M+FA-H-C3H4O4]-, 156.1086[M+FA-H-C5H14O3N]- |  |
| 6 | 2.06 | 312.1089 | C11H21NO7S | N-(1-Deoxy-1-fructosyl)methionine | 312.1133[M+H]+,276.1470[M+H-2H2O]+, 229.1613[M+H-2H2O-CH3S]+ |  |
| 7 | 3.15 | 165.0559 | C9H8O3 | Phenylpyruvic acid | 165.0565[M+H]+, 137.0597[M+H-C2H4]+ |  |
| 8 | 3.18 | 180.0883 | C6H13NO5 | Glucosamine | 180.0923[M+H]+,162.0623[M+H-H2O]+, 144.0488[M+H-2H2O]+ |  |
| 9 | 3.95 | 224.0560 | C9H9NO3 | Adrenochrome | 224.0872[M+FA-H]-, 193.0758[M+FA-H-CH3O]- |  |
| 10 | 5.16 | 338.0888 | C15H17NO8 | 5-Hydroxy-6-methoxyindole glucuronide | 338.0869[M-H]-,175.0228[M-H-C9H9NO2]-, 162.0543[M-H-C6H8O6]- |  |
| 11 | 5.22 | 250.0717 | C11H11NO3 | 5-Methoxyindoleacetate | 250.0707[M+FA-H]-, 206.0789[M+FA-H-CO2]- |  |
| 12 | 5.93 | 146.0607 | C9H7NO | 1H-Indole-3-carboxaldehyde | 146.0629[M+H]+, 119.0891[M+H-CHN]+ |  |
| 13 | 6.04 | 245.1749 | C12H24O2 | Dodecanoic acid | 245.1747[M+FA-H]-, 201.1508[M+FA-H-CO2]-, 173.1205[M+FA-H-C3H4O2]- |  |
| 14 | 6.73 | 333.1129 | C8H9NO3 | Pyridoxal | 333.1052[2M-H]-,297.1392[2M-H-2H2O]-, 283.0883[2M-H-CH6O2]- |  |
| 15 | 7.19 | 321.1579 | C10H11NO | Tryptophanol | 321.1779[2M-H]-,285.1422[2M-H-2H2O]-, 245.1678[2M-H-C3H8O2]- |  |
| 16 | 7.37 | 263.1119 | C10H16N4O3 | Homocarnosine | 263.1129[M+Na]+,245.1223[M+Na-H2O]+, 133.0670[M+Na-C5H8NO3]+ |  |
| 17 | 7.43 | 243.1600 | C12H22O2 | *Trans*-Dodec-2-enoic acid | 243.1411[M+FA-H]-, 113.0649[M+FA-H-C7H14O2]- |  |
| 18 | 7.47 | 593.3384 | C33H44N4O6 | Mesobilirubinogen | 593.8547[M+H]+, 533.3176[M+H-C2H4O2]+ |  |
| 19 | 7.49 | 245.1383 | C12H22O5 | 3-Hydroxydodecanedioic acid | 245.1678[M-H]-,199.1365[M-H-CH2O2]-, 155.1497[M-H-C2H2O4]- |  |
| 20 | 7.80 | 377.0771 | C10H7NO3 | Kynurenic acid | 377.0891[2M-H]-, 243.0661[2M-H-C7H4NO2]-, 233.1867[2M-H-C9H6NO]- |  |
| 21 | 8.09 | 595.3488 | C33H46N4O6 | *L*-Urobilin | 595.3667[M+H]+, 410.1938[M+H-C9H15O3N]+, |  |
| 22 | 8.66 | 327.2318 | C20H32O2 | Arachidonic acid | 327.2346[M+Na]+,291.1256[M+Na-2H2O]+, 267.1656[M+Na-C2H4O2]+ |  |
| 23 | 8.99 | 407.2786 | C24H38O5 | 7-Ketodeoxycholic acid | 407.2189[M+H]+,345.2566[M+H-C2H6O2]+, 315.2454[M+H-C3H8O3]+ |  |
| 24 | 9.02 | 503.2353 | C23H38O7S | 3-Sulfodeoxycholic acid | 503.2355[M+FA-H]-,441.1827[M+FA-H-CH2O3]-, 401.1044[M+FA-H6O4S]- |  |
| 25 | 9.17 | 405.2635 | C24H36O5 | 7a,12a-Dihydroxy-3-oxo-4-cholenoic acid | 405.2651[M+H]+, 290.2769[M+H-C6H11O2]+ |  |