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| --- | --- | --- | --- |
| **Compound Identification** | **General** | **Database Search** | **Library Search** |
| Cpd | Name | Formula | m/z | Mass | Start | RT | End | Score (DB) | Diff (DB, ppm) | Score (Lib) |
| 1 | Sucrose | C12 H22 O11 | 341.1089 | 342.116 | 2.331 | 2.439 | 2.548 | 99.83 | 0.27 | 0 |
| 2 | Symplocoside | C22 H26 O11 | 465.1397 | 466.147 | 5.519 | 5.528 | 5.536 | 98.99 | 1.04 | 0 |
| 3 | Haematoxylin | C16 H14 O6 | 301.0722 | 302.079 | 7.026 | 7.134 | 7.243 | 84.39 | -1.08 | 0 |
| 4 | 1-Naphthyl β-D-glucuronide | C16 H16 O7 | 319.0824 | 320.09 | 7.352 | 7.46 | 7.569 | 98.99 | -0.08 | 0 |
| 5 | Methyl 7-Desoxypurpurogallin-7-Carboxylate Trimethyl Ether | C16 H16 O6 | 303.0884 | 304.096 | 7.704 | 7.762 | 7.821 | 96.44 | -2.78 | 0 |
| 6 | 2',4'-Dihydroxy-2-biphenylcarboxylic acid | C13 H10 O4 | 229.0508 | 230.058 | 8.231 | 8.239 | 8.247 | 99.02 | -1.2 | 0 |
| 7 | 1-Naphthylmethanol glucuronide | C17 H18 O7 | 333.0984 | 334.106 | 8.255 | 8.264 | 8.272 | 98.77 | -0.94 | 0 |
| 8 | 4,7-Dihydroxy-2H-1-benzopyran-2-one | C9 H6 O4 | 177.0196 | 178.027 | 8.407 | 8.465 | 8.524 | 99.39 | -1.23 | 0 |
| 9 | Demethylsulochrin | C16 H14 O7 | 317.0669 | 318.074 | 9.511 | 9.57 | 9.628 | 96.27 | -1.21 | 0 |
| 10 | Machaerol C | C18 H20 O7 | 347.1138 | 348.121 | 9.812 | 9.821 | 9.829 | 99.7 | -0.4 | 0 |
| 11 | Hesperetin | C16 H14 O6 | 301.0718 | 302.079 | 9.837 | 9.908 | 9.979 | 99.12 | -0.06 | 89.14 |
| 12 | Aurasperone A | C32 H26 O10 | 569.1452 | 570.153 | 10.06 | 10.097 | 10.13 | 88.96 | -0.5 | 0 |
| 13 | Phenanthrene-4,5-dicarboxylate | C16 H10 O4 | 265.0505 | 266.058 | 10.44 | 10.511 | 10.58 | 99.13 | 0.5 | 0 |
| 14 | Brazilein | C16 H12 O5 | 283.062 | 284.069 | 10.52 | 10.624 | 10.73 | 96.01 | -2.43 | 92.91 |
| 15 | (±)-Taxifolin | C15 H12 O7 | 303.0513 | 304.059 | 10.67 | 10.674 | 10.68 | 98.98 | -0.54 | 92.03 |
| 16 | Methylnorlichexanthone | C15 H12 O5 | 271.0614 | 272.069 | 10.74 | 10.749 | 10.76 | 98.84 | -0.53 | 88.76 |
| 17 | 3-(3,5-Dihydroxyphenyl)-2-propenoic acid | C9 H8 O4 | 179.0353 | 180.043 | 10.84 | 10.912 | 10.98 | 97.01 | -2.14 | 0 |
| 18 | Urolithin C | C13 H8 O5 | 243.0302 | 244.038 | 11.22 | 11.277 | 11.34 | 99.17 | -1.16 | 0 |
| 19 | Dianhydroaurasperone C | C31 H24 O10 | 601.1357 | 556.137 | 11.62 | 11.628 | 11.64 | 98.6 | -0.42 | 0 |
| 20 | Genistein, 8-Methyl | C16 H12 O5 | 283.0611 | 284.068 | 12.07 | 12.08 | 12.09 | 84.99 | 0.12 | 26.25 |
| 21 | (2S,2''S,3S,3''R,4S)-3,4',5,7-Tetrahydroxyflavan(2->7,4->8)-3,4',5,7-tetrahydroxyflavan | C30 H24 O10 | 603.1509 | 544.137 | 12.12 | 12.181 | 12.24 | 99.71 | 0.03 | 0 |
| 22 | 5,7,3'-Trihydroxy-6,4',5'-trimethoxyflavanone | C18 H18 O8 | 361.093 | 362.1 | 12.67 | 12.682 | 12.69 | 99.29 | -0.17 | 0 |
| **Compound Identification** | **General** | **Database Search** | **Library Search** |
| Cpd | Name | Formula | m/z | Mass | Start | RT | End | Score (DB) | Diff (DB, ppm) | Score (Lib) |
| 23 | Biochanin A | C16 H12 O5 | 283.0615 | 284.069 | 13.18 | 13.285 | 13.39 | 84.62 | -0.86 | 0 |
| 24 | Heliannone C | C16 H14 O5 | 285.077 | 286.084 | 13.43 | 13.486 | 13.54 | 99.37 | -0.54 | 0 |
| 25 | cis-p-Coumaric acid | C9 H8 O3 | 163.0403 | 164.048 | 13.45 | 13.549 | 13.65 | 99.41 | -1.3 | 0 |
| 26 | Isorhamnetin | C16 H12 O7 | 315.0513 | 316.059 | 13.58 | 13.586 | 13.59 | 99.61 | -0.85 | 0 |
| 27 | Rheidin C | C31 H22 O9 | 583.1243 | 538.126 | 13.78 | 13.887 | 14 | 98.66 | 0.47 | 0 |
| 28 | alpha-Peroxyachifolide | C20 H24 O7 | 375.1452 | 376.152 | 13.93 | 13.938 | 13.95 | 99.51 | -0.6 | 0 |
| 29 | p-Hydroxycinnamaldehyde | C9 H8 O2 | 147.045 | 148.052 | 14.08 | 14.088 | 14.1 | 87.52 | 1.24 | 83.03 |
| 30 | Duartin (-) | C18 H20 O6 | 331.1191 | 332.126 | 14.53 | 14.591 | 14.65 | 99.28 | -0.89 | 0 |
| 31 | 6-Hydroxy-6a,12a-dehydro-alpha-toxicarol | C23 H20 O8 | 423.1083 | 424.116 | 14.78 | 14.791 | 14.8 | 99.63 | 0.53 | 0 |
| 32 | Hieracin | C15 H10 O7 | 301.0354 | 302.043 | 14.83 | 14.842 | 14.85 | 99.12 | 0.01 | 88.99 |
| 33 | Physcion | C16 H12 O5 | 283.061 | 284.068 | 14.96 | 14.967 | 14.98 | 85.73 | 0.83 | 88.63 |
| 34 | Palmidin B | C30 H22 O7 | 553.1497 | 494.136 | 15.06 | 15.067 | 15.08 | 91.71 | 0.57 | 0 |
| 35 | Cardamonin | C16 H14 O4 | 269.0822 | 270.089 | 15.74 | 15.796 | 15.85 | 99.1 | -0.67 | 89.35 |
| 36 | 5'-Methoxybilobetin | C32 H22 O11 | 581.1082 | 582.116 | 15.96 | 15.971 | 15.98 | 96.51 | 0.91 | 0 |
| 37 | 9-Methoxy-alpha-lapachone | C16 H16 O4 | 271.0974 | 272.105 | 16.47 | 16.473 | 16.48 | 99.8 | 0.73 |   |
| 38 | Asticolorin C | C33 H28 O9 | 613.1705 | 568.172 | 18.07 | 18.08 | 18.09 | 97.31 | 2.04 | 0 |
| 39 | Gibberellin A3 | C19 H22 O6 | 345.134 | 346.141 | 18.17 | 18.18 | 18.19 | 99.49 | 1.03 | 0 |
| 40 | 5-Hydroxy-7,2',5'-trimethoxyflavone | C18 H16 O6 | 327.0873 | 328.095 | 19.68 | 19.737 | 19.8 | 99.33 | 0.7 | 0 |
| 41 | 7,3',4'-Trihydroxy-3,8-dimethoxyflavone | C17 H14 O7 | 329.067 | 330.074 | 22.37 | 22.423 | 22.48 | 99.32 | -0.64 | 0 |
| 42 | 5,7,4'-Trimethoxyflavone | C18 H16 O5 | 311.0921 | 312.099 | 24.12 | 24.13 | 24.14 | 98.16 | 1.48 | 0 |
| 43 | Dihydromethylsterigmatocystin | C18 H14 O7 | 341.0664 | 342.074 | 24.17 | 24.181 | 24.19 | 98.45 | 0.99 | 0 |
| 44 | Isopalmitic acid | C16 H32 O2 | 255.2328 | 256.24 | 30.4 | 30.457 | 30.52 | 99.65 | 0.53 | 81.94 |
| 45 | Petroselinic acid | C18 H34 O2 | 281.2487 | 282.256 | 31.2 | 31.26 | 31.32 | 85.88 | -0.35 | 59.41 |