Supplementary Table 1 Information of chemical constituents from SR/CSR(n=3)

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No.** | **tR (min)** | **Compounds** | **Chemical Formula** | **CAS No.** | **MW (Da)** | **m/z** | **MS2** | **Relative contents (%)** | **Trend after charring** | **Polarity** |
| **SR** | **CSR** |
| 1 | 9.28  | 1,2,3,6-Tetragalloylglucose | C34H28O22 | 79886-50-3 | 788.1072  | 787.1064  | 169.0154(C7H5O5) | 0.395±0.124 | 0.056±0.002 | ↓↓ | [M-H]- |
| 2 | 10.02  | 1,2,3,4,6-Pentagalloyl-β-D-glucose | C41H32O26 | 14937-32-7 | 940.1182  | 939.1169  | 169.0154(C7H5O5) | 0.214±0.085 | 0.031±0.012 | ↓↓ | [M-H]- |
| 3 | 0.79  | 1-Galloyl-β-glucose | C13H16O10 | 13405-60-2 | 332.0743  | 331.0687  | 301.0589(C12H13O9)169.0158(C7H5O5)112.9867(C4HO4) | 1.548±0.407 | 0.269±0.007 | ↓↓ | [M-H]- |
| 4 | 7.25  | Methoxybenzoic acid methyl ester-5-O-sulfate | C9H10O8S | - | 278.0096  | 277.0040  | 197.0464(C9H9O5) 179.0357(C9H7O4)153.9752(C7H3O4) | 24.683±3.893 | 4.521±3.702 | ↓↓ | [M-H]- |
| 5 | 7.80  | 1,3,6-tris(3,4,5-trihydroxybenzoate)-β-D-Glucopyranose | C27H24O18 | 18483-17-5 | 636.0963  | 635.0880  | 465.0100(C20H17O13) | 0.246±0.091 | 0.054±0.009 | ↓ | [M-H]- |
| 6 | 6.33  | Gallic acid 3-O-β-D-(6'-O-galloyl)-glucopyranoside | C20H20O14 | 87087-61-4 | 484.0853  | 483.0810  | 321.0274(C14H9O9)307.0118(C13H7O9) | 0.611±0.17 | 0.179±0.057 | ↓ | [M-H]- |
| 7 | 5.59  | Chlorogenic acid | C16H18O9 | 327-97-9 | 354.0951  | 353.0779  | 335.0798(C16H15O8) 289.0743(C15H13O6） | 0.102±0.076 | 0.033±0.012 | ↓ | [M-H]- |
| 8 | 2.64  | Methyl 6-O-galloyl-β-D-glucopyranoside | C14H18O10 | 88847-06-7 | 346.0900  | 345.0847  | 169.0124(C7H5O5)112.9868(C4HO4) | 6.569±1.05 | 3.081±1.438 | ↓ | [M-H]- |
| 9 | 5.22  | Glucosyringic acid | C15H20O10 | 33228-65-8 | 360.0156  | 359.0996  | - | 0.09±0.039 | 0.047±0.014 | ↓ | [M-H]- |
| 10 | 7.43  | Ethyl gallate\* | C9H10O5 | 831-61-8 | 198.1730  | 197.0469  | 112.9864(C4HO4) | 4.262±1.302 | 2.858±0.864 | ↓ | [M-H]- |
| 11 | 6.70  | Methyl-6-O-digalloyl-β-D-glucopyranoside/Methyl-4,6-di-O-galloyl-β-D-glucopyranoside | C21H22O14 | - | 498.1010  | 497.0949  | - | 0.383±0.149 | 0.418±0.112 | → | [M-H]- |
| 12 | 4.48  | β-1-O-galloyl-2,3-(S)-hexahydroxydiphenoyl-D-glucose | C27H22O18 | 84316-77-8 | 634.0806  | 633.0747  | 321.0281(C14H9O9)169.0152(C7H5O5)  | 0.122±0.058 | 0.161±0.064 | → | [M-H]- |
| 13 | 7.06  | Brevifolincarboxylic acid | C13H8O8 | 18490-95-4 | 292.0219  | 291.0161  | 112.9900(C4HO4)191.04(C10H7O4) | 0.088±0.032 | 0.121±0.039 | → | [M-H]- |
| 14 | 1.16  | Gallic acid\* | C7H6O5 | 149-91-7 | 170.0215  | 171.0288 | 153.0182(C7H5O4)127.0389(C6H7O3)112.9865(C4HO4） | 4.618±1.952 | 8.309±1.830 | ↑ | [M+H]+ |
| 15 | 5.23  | [Protocatechuic acid](https://www.chemsrc.com/en/cas/99-50-3_1188518.html) | C7H6O4 | 99-50-3 | 154.0226  | 153.0199  | 112.9867(C4HO4) | 0.01±0.007 | 0.083±0.02 | ↑↑ | [M-H]- |
| 16 | 8.54  | Ferulic Acid | C10H10O4 | 1135-24-6 | 194.0579  | 193.0521  | 112.9866(C4HO4) 163.0411(C9H7O3) | 0.004±0.004 | 0.051±0.01 | ↑↑ | [M-H]- |
| 17 | 1.90  | Ethyl 3,4-dihydroxybenzoate | C9H10O4 | 3943-89-3 | 182.0579  | 180.9743  | 125.0264(C6H5O3)153.0538(C8H9O3)169.0146(C8H9O4) | 0.007±0.003 | 0.09±0.004 | ↑↑ | [M-H]- |
| 18 | 10.75  | [Methyl 3,4-methoxy-5-hydroxybenzoate](https://www.chemsrc.com/en/cas/83011-43-2_27689.html) | C10H12O5 | 83011-43-2 | 212.0685  | 213.0757  | 181.0493(C9H9O4) | 0.075±0.023 | 1.259±0.277 | ↑↑ | [M+H]+ |
| 19 | 1.53  | Pyrogallic acid | C6H6O3 | 87-66-1 | 126.0317  | 125.0253  | - | 0.301±0.075 | 5.579±1.509 | ↑↑ | [M-H]- |
| 20 | 8.17  | 3-O-galloylnorbergerin | C20H18O13 | - | 466.0747  | 465.0704  | - | 0.015±0.011 | 0.332±0.064 | ↑↑ | [M-H]- |
| 21 | 4.11  | Methyl gallate\* | C8H8O5 | 99-24-1 | 184.1460  | 183.0311  | 119.0369(C4H7O4)112.9867(C4HO4) | 0.042±0.031 | 5.483±1.343 | ↑↑ | [M-H]- |
| 22 | 13.34  | 3,3',4'-trimethylellagic acid-4-O-sulphate | C17H12O11S | - | 424.0100  | 423.0758  | 408.9888(C16H9O11S) 343.0464(C17H11O8)248.9620(C14HO3S) 112.9867(C4HO4) | 6.348±2.322 | 0.013±0.008 | ↓↓ | [M-H]- |
| 23 | 12.60  | 3,4'-dimethylellagic acid-4-O-sulphate | C16H10O11S | - | 409.9944  | 408.9873  | 329.0326(C16H9O8) 248.9622(C14HO3S) 112.9868(C4HO4) | 7.781±1.267 | 0.198±0.15 | ↓↓ | [M-H]- |
| 24 | 12.23  | 3,4'-di-O-methylellagic acid-4-O-β-D-xylopyranoside | C21H18O12 | 62218-23-9 | 462.0798  | 461.0762  | 112.9870(C4HO4) | 0.384±0.114 | 0.03±0.008 | ↓↓ | [M-H]- |
| 25 | 4.48  | 3,3',4'-tri-O-methylellagic acid-4-O-β-D-xylopyranoside | C22H20O12 | 136133-08-9 | 476.0955  | 475.1057  | 361.0720(C21H17O12)321.0252(C14H9O9) | 0.093±0.045 | 0.027±0.013 | ↓ | [M-H]- |
| 26 | 8.91  | Ellagic acid 4-O-xylopyranoside | C19H14O12 | 139163-18-1 | 434.0485  | 433.0447  | 359.0081(C16H7O10) 112.9868(C4HO4) | 0.028±0.016 | 0.065±0.031 | ↑ | [M-H]- |
| 27 | 15.55  | 3,3',4'-tri-O-methylellagic acid | C17H12O8 | 1617-49-8 | 344.0532  | 343.0480  | 300.9020(C14H5O8)112.9866(C4HO4) | 0.035±0.014 | 0.111±0.031 | ↑ | [M-H]- |
| 28 | 12.60  | 3,4’-O-dimethylellagic acid | C16H10O8 | 57499-59-9 | 330.0376  | 329.0321  | - | 0.083±0.024 | 0.549±0.114 | ↑↑ | [M-H]- |
| 29 | 9.28  | Ellagic acid\* | C14H6O8 | 476-66-4 | 302.0063  | 301.0010  | 137.0253(C7H5O3)112.9865(C4HO4) | 0.392±0.118 | 3.015±0.487 | ↑↑ | [M-H]- |
| 30 | 10.75  | Sanguisorbic acid dilactone | C21H10O13 | 82203-11-0 | 470.0121  | 469.0071  | 300.9996(C14H5O8) | 0.015±0.009 | 0.602±0.079 | ↑↑ | [M-H]- |
| 31 | 2.27  | (-)-Gallocatechin | C15H14O7 | 3371-27-5 | 306.0740  | 307.0812  | 167.0128(C11H3O2)135.0441(C8H7O2) 113.0597(C6H9O2) | 0.180±0.080 | 0.000±0.000 | ↓↓ | [M+H]+ |
| 32 | 5.22  | (-)-Epigallocatechin | C15H14O7 | 970-74-1 | 306.0740  | 307.0812  | - | 0.113±0.024 | 0.000±0.000 | ↓↓ | [M+H]+ |
| 33 | 5.22  | Procyanidin B3 (Catechin dimer) | C30H26O12 | 23567-23-9 | 578.1424  | 577.1359  | 289.0743(C15H13O6) 305.0682(C15H13O7) | 3.312±0.764 | 0.232±0.131 | ↓↓ | [M-H]- |
| 34 | 8.17  | 3-O-galloylprocyanidin B3 (Derivative of catechin dimer) | C37H30O16 | 73086-04-1 | 730.1534  | 729.1497  | 577.1375(C30H25O12)  | 5.181±1.484 | 0.380±0.201 | ↓↓ | [M-H]- |
| 35 | 3.01  | Procyanidin | C30H26O13 | 4852-22-6 | 594.1373  | 593.1330  | 345.0864(C16H9O9)313.0582(C13H13O9) 112.9863(C4HO4) | 0.468±0.173 | 0.036±0.026 | ↓↓ | [M-H]- |
| 36 | 5.59  | Procyanidin C2 (Catechin trimer) | C45H38O18 | 37064-31-6 | 866.2058  | 865.2011  | 579.1542(C30H27O12) 357.0616(C18H13O8) 325.0508(C21H9O4) 289.0743(C15H13O6) | 0.435±0.152 | 0.041±0.032 | ↓↓ | [M-H]- |
| 37 | 5.59  | Catechin\* | C15H14O6 | 154-23-4 | 290.2680  | 289.0736  | 193.0104(C9H5O5)165.0183(C8H5O4) 137.0252(C7H5O3)112.9867(C4HO4) | 9.674±1.416 | 1.100±0.573 | ↓↓ | [M-H]- |
| 38 | 7.80  | Fisetinidol (4β→8)-catechin | C30H26O11 | [57526-59-7](https://www.chemsrc.com/baike/244844.html) | 562.1475  | 561.1439  | 317.0430(C17H17O6)289.0713(C15H13O6)227.0047(C5H7O10) | 0.315±0.153 | 0.053±0.017 | ↓↓ | [M-H]- |
| 39 | 9.28  | [(-)-Epicatechin gallate](https://www.chemsrc.com/en/cas/1257-08-5_598585.html) | C22H18O10 | [1257-08-5](https://www.chemsrc.com/baike/598585.html) | 442.0900  | 441.0846  | 287.0564(C15H11O6) 169.0151(C7H5O5) 112.9865(C4HO4) | 0.144±0.048 | 0.033±0.006 | ↓ | [M-H]- |
| 40 | 3.38 | Protocatechualdehyde | C7H6O3 | 139-85-5 | 138.0317 | 137.0251 | 112.9864(C4HO4)  | 0.105±0.014 | 2.084±0.812 | ↑↑ | [M-H]- |

\* marked after compound name means mass spectrum of the compound has been identified with that of corresponding standard.

“↑” means FC≥1.5, and “↑↑” means FC≥5. “↓” means FC≤0.67, and “↓↓” means FC≤0.2. “→” means 0.67<FC<1.5.