

Supplemental File S7: Summarized compound list with further analytical data

Table G1: compound list with further analytical data

| nr. | Compound | group | RT (min) | Precursor ion (<i>m/z</i>) | Adduct | CCS (Å ²) | Characteristic mass fragments (<i>m/z</i>) |
|-----|--|-----------------------|----------|------------------------------|--------|-----------------------|--|
| 1a | hydrangenol 8-O-glucoside (isomer 1) | dihydroisocoumarin | 4.37 | 417.1199 | -H | 199.54 | 255.0656 (C ₁₅ H ₁₁ O ₄ ⁻), 211.0761 (C ₁₄ H ₁₁ O ₂ ⁻) |
| 1b | hydrangenol 8-O-Glc (isomer 2) | dihydroisocoumarin | 4.63 | 417.1194 | -H | 201.51 | 255.0656 (C ₁₅ H ₁₁ O ₄ ⁻), 211.0761 (C ₁₄ H ₁₁ O ₂ ⁻) |
| 2a | thunberginol G-3'-O-Glc (isomer 1) | dihydroisocoumarin | 5.74 | 433.1139 | -H | 195.57 | 271.0606 (C ₁₅ H ₁₁ O ₅ ⁻), 227.0709 (C ₁₄ H ₁₁ O ₃ ⁻) |
| 2b | thunberginol G-3'-O-Glc (isomer 2) | dihydroisocoumarin | 5.82 | 433.1145 | -H | 189.44 | 271.0606 (C ₁₅ H ₁₁ O ₅ ⁻), 227.0709 (C ₁₄ H ₁₁ O ₃ ⁻) |
| 3a | phyllodulcin-8-O-Glc (isomer 1) | dihydroisocoumarin | 4.88 | 447.1296 | -H | 194.74 | 285.0767 (C ₁₆ H ₁₃ O ₅ ⁻), 241.0869 (C ₁₅ H ₁₃ O ₃ ⁻), 225.0556 (C ₁₄ H ₉ O ₃ ⁻) |
| 3b | phyllodulcin-8-O-Glc (isomer 2) | dihydroisocoumarin | 5.13 | 447.1295 | -H | 194.83 | 285.0767 (C ₁₆ H ₁₃ O ₅ ⁻), 241.0869 (C ₁₅ H ₁₃ O ₃ ⁻), 225.0556 (C ₁₄ H ₉ O ₃ ⁻) |
| 4 | hydrangenol-4'-O-Glc | dihydroisocoumarin | 5.97 | 417.1187 | -H | 216.86 | 255.0658 (C ₁₅ H ₁₁ O ₄ ⁻), 211.0760 (C ₁₄ H ₁₁ O ₂ ⁻) |
| 5 | phyllodulcin-3'-O-Glc | dihydroisocoumarin | 6.23 | 447.1298 | -H | 191.87 | 285.0763 (C ₁₆ H ₁₃ O ₅ ⁻), 241.0865 (C ₁₅ H ₁₃ O ₃ ⁻), 225.0551 (C ₁₄ H ₉ O ₃ ⁻) |
| 6 | thunberginol C-8-O-glucoside | dihydroisocoumarin | 4.04 | 433.1141 | -H | 190.26 | 271.0607 (C ₁₅ H ₁₁ O ₅ ⁻), 227.0712 (C ₁₄ H ₁₁ O ₃ ⁻) |
| 7 | thunberginol E-6-O-glucoside | dihydroisocoumarin | 4.95 | 463.1256 | -H | 195.82 | 301.0718 (C ₁₆ H ₁₃ O ₆ ⁻), 257.0817 (C ₁₅ H ₁₃ O ₄ ⁻), 241.0504 (C ₁₄ H ₉ O ₄ ⁻) |
| 8 | thunberginol D-6-glucoside | dihydroisocoumarin | 3.78 | 449.1091 | -H | 191.28 | 287.0555 (C ₁₅ H ₁₁ O ₆ ⁻), 269.0447 (C ₁₅ H ₉ O ₅ ⁻), 243.0656 (C ₁₄ H ₁₁ O ₃ ⁻) |
| 9 | thunberginol C | dihydroisocoumarin | 6.3 | 271.0627 | -H | 163.02 | 227.0724 (C ₁₄ H ₁₁ O ₃ ⁻) |
| 10 | thunberginol E | dihydroisocoumarin | 6.69 | 301.0721 | -H | 173.81 | 283.0628 (C ₁₆ H ₁₁ O ₅ ⁻), 257.0834 (C ₁₅ H ₁₃ O ₄ ⁻), 241.0518 (C ₁₄ H ₉ O ₄ ⁻) |
| 11 | thunberginol G | dihydroisocoumarin | 7.04 | 271.0610 | -H | 156.29 | 227.0711 (C ₁₄ H ₁₁ O ₃ ⁻) |
| 12 | hydrangenol | dihydroisocoumarin | 8.15 | 255.0675 | -H | 160.24 | 211.0767 (C ₁₄ H ₁₁ O ₂ ⁻) |
| 13 | phyllodulcin | dihydroisocoumarin | 8.39 | 285.0769 | -H | 171.41 | 225.0555 (C ₁₄ H ₉ O ₃ ⁻) |
| 14 | cudrabilbenzyl A | dihydrostilbenic acid | 3.62 | 436.1337 | -H | 196.52 | 273.0765 (C ₁₅ H ₁₃ O ₅ ⁻), 255.0658 (C ₁₅ H ₁₁ O ₄ ⁻), 229.0868 (C ₁₄ H ₁₃ O ₃ ⁻), 123.0451 (C ₇ H ₇ O ₂ ⁻) |
| 15 | 2,4-Dihydroxy-6-[2-(-hydroxyphenyl)]benzoic acid | dihydrostilbenic acid | 5.84 | 273.0785 | -H | 163.00 | 255.0675 (C ₁₅ H ₁₁ O ₄ ⁻), 229.0801 (C ₁₄ H ₁₃ O ₃ ⁻), 123.0457 (C ₇ H ₇ O ₂ ⁻) |
| 16 | lunularin-4'-glucoside | dihydrostilbene | 5.68 | 375.1454 | -H | 180.32 | 213.0919 (C ₁₄ H ₁₃ O ₂ ⁻), 107.0500 (C ₇ H ₇ O ⁻) |
| 17 | dihydroresveratrol-3-O-glucoside | dihydrostilbene | 4.39 | 391.1401 | -H | 185.77 | 229.0867 (C ₁₄ H ₁₃ O ₃ ⁻), 123.0449 (C ₇ H ₇ O ₂ ⁻) |
| 18 | 4-Hydroxy-8-(4-glucopyranosyl)hydroxyphenyl)octane-2,6-dione | triketide | 3.15 | 411.1656 | -H | 199.00 | 393.1551 (C ₂₀ H ₂₅ O ₈ ⁻), 353.1236 (C ₁₇ H ₂₁ O ₈ ⁻), 231.1017 (C ₁₄ H ₁₅ O ₃ ⁻), 191.0706 (C ₁₁ H ₁₁ O ₃ ⁻) |
| 19 | taxiphyllin | cyanogenic glycoside | 2.05 | 310.0924 | -H | 240.37 | 179.0557 (C ₆ H ₁₁ O ₆ ⁻) |
| 20 | deoxyloganic acid | secoiridoid | 4.04 | 359.1345 | -H | 183.24 | 197.0814 (C ₁₀ H ₁₃ O ₄ ⁻), 153.0916 (C ₉ H ₁₃ O ₂ ⁻), 135.0812 (C ₉ H ₁₂ O ⁻) |

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| 21 | loganic acid | secoiridoid | 2.59 | 375.1297 | -H | 186.21 | 195.0653 (C ₁₀ H ₁₁ O ₄ ⁻), 151.0759 (C ₉ H ₁₁ O ₂ ⁻) |
| 22 | hydramacroside B | secoiridoid | 5.59 | 605.2258 | -H | 236.88 | 587.2147 (C ₃₀ H ₃₅ O ₁₂ ⁻), 441.1409 (C ₂₀ H ₂₅ O ₁₁ ⁻), 413.1458 (C ₁₉ H ₂₅ O ₁₀ ⁻) |
| 23 | hydrangenoside A | secoiridoid | 6.33 | 619.2397 | -H | 239.42 | 601.2286 (C ₃₁ H ₃₇ O ₁₂ ⁻), 231.1018 (C ₁₄ H ₁₅ O ₃ ⁻), 189.0914 (C ₁₂ H ₁₃ O ₂ ⁻) |
| 24 | quercetin-3-O-rhamnopyransyl sophoroside | flavonol | 3.63 | 771.2013 | -H | 258.12 | 300.0268 (C ₁₅ H ₈ O ₇ ⁻) |
| 25 | quercetin-3-O-sophoroside | flavonol | 3.76 | 625.1424 | -H | 231.49 | 300.0274 (C ₁₅ H ₈ O ₇ ⁻) |
| 26 | kaempferol-3-O-sophoroside | flavonol | 4.15 | 609.1466 | -H | 231.03 | 284.0317 (C ₁₅ H ₈ O ₆ ⁻) |