**Suppl. Table S1.** Metabolites identified in 100 % methanol extract of *Prunus mahaleb* L. seed cvs. using UPLC-ESI-MS in negative and positive ionization modes

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No** | **Rt** | **Compound**  **name** | **Chemical class** | **[M-H]-/**  **[M+H]+** | **Formula** | **Error**  **ppm** | **MS/MS** | **EGM** | **WEM** | **REM** | **RREM** |
| 1 | 0.532 | Arginine | Amino acid | 175.1196 | C6H15N4O2+ | 3.69 | 158, 130 | + | + |  |  |
| 2 | 0.571 | Choline | *N*-Trimethylated amino acid | 104.1075 | C5H15NO+ | 6.46 | 60 | + | + | + | + |
| 3 | 0.585 | Sugar alcohol | Sugar | 181.0722 | C6H13O6- | 2.11 | 59 | + | + |  | + |
| 4 | 0.629 | Sucrose | Sugar | 341.1091 | C12H21O11- | 0.29 | 195, 75 | + | + |  | + |
| 5 | 0.638 | Gluconic acid | Organic acid | 195.051 | C6H11O7- | 0.05 | 89, 71, 59 | + |  | + |  |
| 6 | 0.642 | Hexosyl-pentahydroxyheptanoic acid | Hydroxylated fatty acid | 387.1144 | C13H23O13- | 0.36 | 341, 179, 119, 89 | + | + |  | + |
| 7 | 0.651 | Dihydroxy phenol galloyl hexoside | Polyphenol | 439.0857 | C19H19O12- | 3.35 | 332, 96 |  |  | + | + |
| 8 | 0.662 | Malic acid | Organic acid | 133.0145 | C4H5O5- | 0.88 | 96 |  | + | + | + |
| 9 | 0.76 | Unknown | -- | 112.087 | C5H10N3+ | 1.19 | 95, 78, 51 |  |  |  | + |
| 10 | 0.854 | Pyroglutamic acid | Amino acid | 130.05 | C5H8NO3+ | 1.43 | 57 | + | + | + | + |
| 11 | 0.855 | Nicotinic acid | Amino acid | 124.0393 | C6H6NO2+ | 2 | 80, 53 | + | + |  |  |
| 12 | 0.856 | Citric acid | Organic acid | 191.0197 | C6H7O7- | 0.14 | 111, 87 | + | + | + | + |
| 13 | 0.86 | Lactic acid | Organic acid | 89.0244 | C3H5O3- | 0.17 | 68 |  |  | + |  |
| 14 | 0.896 | Adenosine | Amino acid | 268.1041 | C10H14N5O4+ | 0.22 | 136, 57 | + | + | + | + |
| 15 | 0.9 | Tyrosine | Amino acid | 182.0811 | C9H12NO3+ | 0.13 | 91, 77 | + | + | + |  |
| 16 | 0.946 | Isoleucine | Amino acid | 132.1019 | C6H14NO2+ | 0.26 | 86, 69 | + | + | + | + |
| 17 | 0.976 | Glutaryl carnitine | Acyl carnitine | 276.1443 | C12H22NO6+ | 0.54 | 258, 230, 212, 86 |  | + | + |  |
| 18 | 0.978 | Succinic acid | Organic acid | 117.0194 | C4H5O4- | 0.82 | 95, 73 |  |  | + | + |
| 19 | 1.002 | Deoxy fructosyl leucine | Amino acid derivative | 294.1547 | C12H24NO7+ | 0.2 | 276, 258, 230, 86 |  |  | + |  |
| 20 | 1.517 | Phenylalanine | Amino acid | 166.0865 | C9H12NO2+ | 1.46 | 120, 103, 51 | + | + | + | + |
| 21 | 1.567 | Unknown auxin derivative | Auxin | 368.0984 | C16H18NO9- | 0.96 | 328, 257, 144, 59 | + | + |  |  |

**Table 1.** continued

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No** | **Rt** | **Compound name** | **Chemical class** | **[M-H]-/**  **[M+H]+** | **Formula** | **Error**  **ppm** | **ms/ms** | **EGM** | **WEM** | **REM** | **RREM** |
| 22 | 1.616 | Unknown | -- | 146.0602 | C9H8NO+ | 0.89 | 128, 91, 51 | + | + |  |  |
| 23 | 1.709 | Unknown | -- | 358.1145 | C15H20NO9- | 0.28 | 150, 71 | + | + |  |  |
| 24 | 1.715 | Unknown | -- | 134.0603 | C8H8NO+ | 1.7 | 106, 79, 51 | + | + | + |  |
| 25 | 1.747 | Unknown | -- | 649.2209 | C24H41O20+ | 3.29 | 336, 174 | + |  |  |  |
| 26 | 1.991 | Unknown | -- | 297.1558 | C12H25O8+ | 0.14 | 192, 132, 88 |  |  |  | + |
| 27 | 2.228 | Unknown | -- | 188.0711 | C11H10NO2+ | 1.28 | 146, 74 | + | + | + |  |
| 28 | 2.407 | Coumaric acid-*O*- dihexoside | Hydroxycinnamtes | 487.1454 | C21H27O13- | 0.91 | 256, 163, 119 | + | + |  |  |
| 29 | 2.435 | Unknown amino sugar | Amino acid derivative | 506.1867 | C21H32NO13+ | 0.18 | 289,165, 85 | + | + |  |  |
| 30 | 2.475 | Unknown | -- | 582.2395 | C24H40NO15+ | 0.15 | 448, 297, 107 |  |  | **+** |  |
| 31 | 2.526 | Unknown nitrogenous compound | Nitrogenous compound | 102.0914 | C5H12NO+ | 0 | 57 | + |  |  |  |
| 32 | 2.618 | Unknown | -- | 146.1174 | C7H16NO2+ | 0.03 | 57 | + |  |  |  |
| 33 | 2.658 | Unknown | -- | 447.15 | C19H27O12- | 2.44 | 299, 192, 133 |  |  | **+** |  |
| 34 | 2.665 | Unknown | -- | 420.1863 | C18H30NO10+ | 0.36 | 343, 223, 107 |  |  | **+** |  |
| 35 | 2.717 | Unknown | -- | 450.1972 | C19H32NO11+ | 0.76 | 217, 91 | + | + | **+** | **+** |
| 36 | 2.81 | Unknown | -- | 651.1844 | C37H31O11- | 0.35 | 573, 423, 325, 163, 119 | + |  |  | **+** |
| 37 | 2.824 | Tyrosinyl hexoside. | Amino acid derivative | 344.1215 | C15H22NO8+ | 0.76 | 165, 147 | + | + | **+** | **+** |
| 38 | 2.847 | *p*-Coumaric acid | Hydroxycinnamtes | 165.0548 | C9H9O3+ | 1.25 | 119 | + | + |  |  |
| 39 | 2.855 | *p*-Coumaric acid-*O*-hexoside | Hydroxycinnamtes | 325.0785 | C15H17O8- | 2.95 | 277, 163, 119, 59 | + | + | **+** | **+** |
| 40 | 2.86 | Phenylacetaldehyde | Phenyl propane aldehyde | 119.0509 | C8H7O- | 5.52 | 59 | + |  | **+** |  |

**Table 1.** continued

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No** | **Rt** | **Compound name** | **Chemical class** | **[M-H]-/**  **[M+H]+** | **Formula** | **Error**  **ppm** | **ms/ms** | **EGM** | **WEM** | **REM** | **RREM** |
| 41 | 2.943 | Unknown | -- | 489.1525 | C28H25O8- | 1.33 | 165, 121 | + | + |  |  |
| 42 | 3.031 | Methoxy hydroxy amygdalin | Cyanogenic glycoside | 502.1559 | C21H28NO13- | 1.62 | 456, 325, 221, 178, 59 | + | + | **+** | **+** |
| 43 | 3.04 | Unknown | -- | 475.1923 | C20H31N2O11+ | 0.02 | 145 | + | + | **+** | **+** |
| 44 | 3.047 | Amygdalin | Cyanogenic glycoside | 456.1505 | C20H26NO11- | 1.62 | 323, 263, 221 |  |  | **+** | **+** |
| 45 | 3.237 | Unknown | -- | 519.1712 | C22H31O14- | 0.66 | 195, 151, 59 |  | + |  |  |
| 46 | 3.29 | Norharman | *β*-Carboline | 169.076 | C11H7N2- | 0.05 | 115 |  |  |  | **+** |
| 47 | 3.329 | Unknown | -- | 230.1177 | C14H16NO2+ | 0.43 | 91 |  |  | **+** | **+** |
| 48 | 3.342 | Ferulic acid-*O*-hexoside dimer | Hydroxycinnamtes | 711.2147 | C32H39O18- | 0.38 | 355, 193, 59 | + | + | **+** |  |
| 49 | 3.401 | Vanillin | Phenolic aldehyde | 153.0548 | C8H9O3+ | 1.17 | 125 | + | + |  |  |
| 50 | 3.496 | Hydroxybenzaldehyde | Phenyl propane | 121.0294 | C7H5O2- | 1.22 | 92, 77 |  |  | **+** | **+** |
| 51 | 3.532 | Dihydrocoumaroyl-*O*- hexoside (Dihydromelilotoside) | Hydroxycinnamtes | 327.1082 | C15H19O8- | 1.08 | 259, 165, 121 | + | + |  |  |
| 52 | 3.536 | Unknown amino sugar | Amino sugar | 346.1498 | C15H24NO8+ | -0.41 | 215, 149 | + | + |  |  |
| 53 | 3.541 | Dihydrocoumaroyl-*O*- hexoside dimer | Hydroxycinnamtes | 655.2164 | C30H39O16- | 0.82 | 327, 165, 121 | + | + |  |  |
| 54 | 3.687 | Unknown | -- | 340.1034 | C15H18NO8- | 1.23 | 284, 71 |  |  |  | **+** |
| 55 | 3.86 | Hexosyl methoxyphenyl propanoic acid | Hydroxycinnamtes | 357.1186 | C16H21O9- | 1.63 | 195, 151 | + | + |  |  |
| 56 | 3.876 | Dihydroferulic acid-*O*- hexoside dimer | Hydroxycinnamtes | 715.2462 | C32H43O18- | 0.13 | 621, 357, 195 | + | + |  |  |
| 57 | 3.884 | Unknown | -- | 376.1603 | C16H26NO9+ | 0.01 | 179, 55 | + | + |  |  |
| 58 | 4.263 | Ferulic acid-*O*-hexoside | Hydroxycinnamtes | 355.1033 | C16H19O9- | 0.63 | 193,134, 59 | + | + | **+** | **+** |

**Table 1.** continued

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No** | **Rt** | **Compound name** | **Chemical class** | **[M-H]-/**  **[M+H]+** | **Formula** | **Error**  **ppm** | **ms/ms** | **EGM** | **WEM** | **REM** | **RREM** |
| 59 | 4.29 | Ferulic acid | Hydroxycinnamtes | 195.0652 | C10H11O4+ | 0.08 | 177 | + | + | **+** | **+** |
| 60 | 4.411 | Unknown | -- | 573.9756 | C22H8NO13- | 1.8 | 522, 412, 161 | + |  |  |  |
| 61 | 4.423 | Unknown | -- | 700.0299 | C36H15NO13P- | 1.59 | 692, 539, 161 |  |  |  | **+** |
| 62 | 4.483 | Apigenin-*C*-hexoside | Flavonoid | 431.0972  433.1128 | C21H19O10-  C21H21O10+ | 1.31  0.44 | 341, 311, 283, 269  343, 313, 283, 271 |  |  | **+** |  |
| 63 | 4.648 | Prupersin E | Cyanogenic glycoside | 563.1878 | C26H31N2O12+ | 0.84 | 430, 268, 124 |  |  | **+** | **+** |
| 64 | 4.726 | Flavone (luteolin)-methoxy-*C*-hexoside | Flavonoid | 461.1087  463.1234 | C22H21O11-  C22H23O11+ | 1.26  0.37 | 371, 341, 298  373, 343 |  |  | **+** |  |
| 65 | 4.922 | Caffeyl alcohol | Hydroxycinnamtes | 165.0557 | C9H9O3- | 0.18 | 147, 121 |  | + |  |  |
| 66 | 5.226 | Dihydroferulic acid | Hydroxycinnamtes | 195.006 | C10H11O4- | 0.16 | 136,121 | + | + |  |  |
| 67 | 5.424 | Unknown | -- | 187.0975 | C9H15O4- | 0.32 | 212 | + | + | **+** |  |
| 68 | 5.858 | Unknown | -- | 739.3533 | C37H55O15- | 1.93 | 605, 513, 321 |  |  | **+** |  |
| 69 | 5.92 | Coumarin | Coumarin | 147.0442 | C9H7O2+ | 0.8 | 132, 119, 103, 91 | + | + | **+** | **+** |
| 70 | 6.39 | Unknown | -- | 497.2899 | C30H41O6+ | 0.43 | 482, 349, 209, 104 |  |  | **+** |  |
| 71 | 6.41 | Unknown | -- | 721.3436 | C37H53O14- | 0.99 | 675, 596, 495, 321 |  |  | **+** |  |
| 72 | 6.44 | Unknown | -- | 499.3056 | C30H43O6+ | 0.24 | 481, 317, 167, 113 |  |  | **+** |  |
| 73 | 6.96 | Methoxy coumarin (herniarin) | Coumarin | 177.0548 | C10H9O3+ | 2.67 | 162, 133, 121, 85 | + | + | **+** | **+** |
| 74 | 7.981 | Unknown | -- | 170.1542 | C10H20NO+ | 1.54 | 142, 112, 86, 57 | + |  |  |  |
| 75 | 8.077 | Unknown | -- | 736.3905 | C38H58NO13+ | -0.8 | 341, 161, 74 |  | + |  |  |
| 76 | 8.284 | Unknown | -- | 738.1059 | C38H60NO13+ | 0.5 | 335, 241, 113 |  | + |  |  |
| 77 | 8.561 | Unknown | -- | 376.1755 | C20H26NO6+ | 0.04 | 253, 91 | + | + |  |  |
| 78 | 9.204 | Nonamide | Fatty acyl amide | 158.1543 | C9H20NO+ | 2.13 | 57 | + | + | **+** | **+** |
| 79 | 9.57 | Decanamide | Fatty acyl amide | 172.1695 | C10H22NO+ | 0.51 | 121, 116, 74, 60 |  |  | **+** |  |

**Table 1.** continued

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No** | **Rt** | **Compound name** | **Chemical class** | **[M-H]-/**  **[M+H]+** | **Formula** | **Error**  **ppm** | **ms/ms** | **EGM** | **WEM** | **REM** | **RREM** |
| 80 | 10.657 | Unknown | -- | 309.2067 | C18H29O4- | 1.59 | 291, 209, 99 |  | + |  |  |
| 81 | 10.68 | Oxo-octadecatrienoic acid | Fatty acid | 293.2117 | C18H29O3+ | 1.39 | 275, 237, 197, 137 | + | + |  |  |
| 82 | 10.886 | Unknown | -- | 286.1441 | C17H18NO3- | 0.99 | 201, 135, 69 |  | + |  |  |
| 83 | 11.414 | Unknown | -- | 574.338 | C32H48NO8+ | 1.1 | 497, 385, 219, 111 |  |  | **+** |  |
| 84 | 11.565 | Benzyl tetradecanamine | Arylalkylamine | 304.3001 | C21H38N+ | 0.71 | 212, 91 | + | + | **+** | **+** |
| 85 | 11.747 | Unknown | -- | 415.2117 | C24H31O6+ | 0.49 | 296, 119 | + | + | **+** | **+** |
| 86 | 11.824 | Unknown oxylipid | Oxylipid | 307.1913 | C18H27O4- | 0.76 | 223, 137, 99 |  | + |  |  |
| 87 | 12.898 | Nonadecanamine | Amino lipid | 284.3311 | C19H42N+ | 0.42 | 202, 60 | + | + | **+** | **+** |
| 88 | 12.931 | Unknown | -- | 476.2773 | C30H40NO4+ | 2.15 | 279, 196 |  | + |  |  |
| 89 | 12.972 | Benzyl hexadecanamine | Arylalkylamine | 332.3314 | C23H42N+ | 0.59 | 240, 91 | + | + | **+** | **+** |
| 90 | 13.11 | Unknown | -- | 520.3404 | C28H46N3O6+ | 1.42 | 258, 184 |  | + | **+** | **+** |
| 91 | 13.129 | Unknown sphingolipid | Shingolipid | 564.3296 | C27H51NO9P- | 2.24 | 279 |  | + | **+** | **+** |
| 92 | 13.78 | Unknown | -- | 496.3402 | C26H46N3O6+ | 1.57 | 419, 258, 184 |  | + | **+** | **+** |
| 93 | 14.22 | Unknown sphingolipid | Shingolipid | 522.356 | C26H51NO7P- | 1.07 | 279, 196 |  |  | **+** | **+** |
| 94 | 14.288 | Heptanamine | Amino lipid | 312.3626 | C21H46N+ | 0.27 | 224, 60 | + | + |  |  |
| 95 | 14.304 | Unknown sphingolipid | Shingolipid | 566.3453 | C27H53NO9P- | 2.08 | 281, 78 |  | + | **+** | **+** |
| 96 | 14.371 | Stearidonic acid | Fatty acid | 277.2164 | C18H29O2+ | 0.48 | 133 | + | + |  |  |
| 97 | 14.31 | Benzyl  octadecylamine | Arylalkylamine | 360.2636 | C25H46N+ | 0.04 | 268, 91 | + | + | **+** | **+** |
| 98 | 14.321 | Unknown | -- | 595.2878 | C34H43O9- | 5.85 | 456, 265,115 |  | + | **+** |  |
| 99 | 14.619 | Hydroxylinoleic acid | Fatty acid | 295.2268 | C18H31O3+ | 0.26 | 277, 195 | + |  |  |  |
| 100 | 15.088 | Benzofurandione | Benzofuran | 149.0237 | C8H5O3+ | -2.2 | 57 |  | + | **+** |  |

**Table 1.** continued

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No** | **Rt** | **Compound name** | **Chemical class** | **[M-H]-/**  **[M+H]+** | **Formula** | **Error**  **ppm** | **ms/ms** | **EGM** | **WEM** | **REM** | **RREM** |
| 101 | 15.795 | Linaloyl ethanolamide | Fatty ethanolamide | 324.2898 | C20H38NO2+ | 0.04 | 306, 62 | + | + |  |  |
| 102 | 16.606 | Palmitoyl ethanolamide | Fatty ethanolamide | 300.2898 | C18H38NO2+ | -0.16 | 283, 62 | + |  |  |  |
| 103 | 17.184 | Oleoyl ethanolamide | Fatty ethanolamide | 326.3055 | C30H40NO2+ | -0.31 | 309, 62 | + |  |  |  |
| 104 | 17.684 | Unknown oxylipid | Oxylipid | 377.1422 | C23H21O5- | -6.35 | 217, 99 |  | + |  |  |
| 105 | 17.699 | Octadecenedioic acid | Fatty acid | 311.2229 | C18H31O4- | 0.05 | 293, 171 |  | + |  |  |
| 106 | 18.277 | Unknown oxylipid | Oxylipid | 379.1581 | C23H23O5- | -6.89 | 230, 99 |  | + | **+** |  |
| 107 | 18.295 | Unknown | -- | 325.2381 | C19H33O4- | 1.15 | 307, 225, 113 |  | + |  |  |
| 108 | 19.518 | Unknown oxylipid | Oxylipid | 381.1731 | C23H25O5- | -5.56 | 289, 198, 99 |  | + |  |  |
| 109 | 19.541 | Unknown steroid | Steroid | 327.2539 | C30H53O7- | 1.39 | 410, 281 | + | + |  |  |
| 110 | 21.268 | Docosenamide | Fatty acyl amide | 338.3413 | C22H44NO+ | 0.17 | 321, 303, 233, 57 | + | + | **+** |  |