**Supplementary material**

Table S1. Lists the metabolites detected in raw compounds from all samples at the MS1 and MS2 levels.

Positive mode

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No** | **RT (min)** | **Metabolite name** | **Formula** | **Ontology** | **Precursor type** | **Precursor mz** | **MS/MS spectrum** | **Mass error** |
| 1 | 20.92 | Humulene (alpha) | C15H24 | Sesquiterpenoids | [M+H]+ | 205.1945 | 81.06994, 121.10103,149.13309, 203.17834, 205.1958 | 0.0005772 |
| 2 | 28.77 | Prespatane | C15H24 | - | [M+H]+ | 205.1944 | 81.0705, 121.10104, 149.13319, 205.19589 | 0.0006772 |
| 3 | 17.33 | (2R)-2-[(2R,5S)-5-[(2S)-2-hydroxybutyl]oxolan-2-yl]propanoic acid | C11H20O4 | Oxolanes | [M+H]+ | 217.1424 | 55.05494, 97.1011, 125.0965, 217.14284 | 0.0010356 |
| 4 | 12.37 | 3-Hydroxy-5-isopropylidene-3,8-dimethyl-2,3,3a,4,5,8a-hexahydro-6(1H)-azulenone | C15H22O2 | Guaianes | [M–H2O+H]+ | 217.1583 | 105.07006, 131.08551, 199.14771, 217.1588 | 0.0003917 |
| 5 | 13.87 | 2(1H)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-6-hydroxy-3,8-dimethyl-5-(1-methylethyl)-, (4aR,5S,6S,8R,8aS)- | C15H24O2 | Sesquiterpenoids | [M–H2O+H]+ | 219.1741 | 83.08607, 123.11654, 145.10065, 201.16397, 202.16608, 219.17516 | 0.0002418 |
| 6 | 11.57 | Muurolladie-3-One | C15H22O | Sesquiterpenoids | [M+H]+ | 219.1737 | 67.05479, 81.06997, 95.08588, 119.0854, 147.11578, 161.13289, 175.14807, 219.17532 | 0.0006418 |
| 7 | 20.86 | 1,8-Azulenediol, 1,2,3,3a,4,7,8,8a-octahydro-3a,6-dimethyl-1-(1-methylethyl)-, (1R,3aR,8S,8aS)- | C15H26O2 | Sesquiterpenoids | [M–H2O+H]+ | 221.1889 | 95.04995, 147.11732, 203.17912, 221.18999 | 0.0010918 |
| 8 | 8.71 | Unknown-1 | C15H22O3 | - | [M–H2O+H]+ | 233.1535 | 59.0495, 85.02855, 105.96308, 125.0594, 217.15863, 233.1879 | 0.0001063 |
| 9 | 16.45 | 2-[(1S,2S,4aR,8aS)-1-Hydroxy-4a-methyl-8-methylenedecahydro-2-naphthalenyl]acrylic acid | C15H22O3 | Eudesmane, isoeudesmane or cycloeudesmane sesquiterpenoids | [M–H2O+H]+ | 233.153 | 67.05479, 105.96325, 119.08567, 145.10106, 159.08087, 187.14857, 215.1424, 233.18828 | 0.0006063 |
| 10 | 14.06 | 7,8-Bis(hydroxymethyl)-1,4a-dimethyl-3,4,4a,5,6,7-hexahydro-2H-benzo[7]annulen-2-one | C15H22O3 | Cyclohexenones | [M–H2O+H]+ | 233.1529 | 105.96307, 131.08524, 173.13199, 215.14211, 233.18785 | 0.0007063 |
| 11 | 19.48 | Curcumeno | C15H22O2 | Guaianes | [M+H]+ | 235.1684 | 133.10149, 189.16315, 217.15926, 235.20467 | 0.0008564 |
| 12 | 26.58 | 2-[(2R,4aR,8R,8aR)-8-Hydroxy-4a,8-dimethyldecahydro-2-naphthalenyl]acrylic acid | C15H24O3 | Eudesmane, isoeudesmane or cycloeudesmane sesquiterpenoids | [M–H2O+H]+ | 235.1686 | 95.08575, 133.10091, 147.11734, 175.14766, 189.12769, 217.19417, 235.20578 | 0.0006564 |
| 13 | 18.37 | (4aR,5R,6R)-6-Hydroxy-3-isopropylidene-4a,5-dimethyl-4,4a,5,6,7,8-hexahydro-2(3H)-naphthalenone | C15H22O2 | Eremophilane, 8,9-secoeremophilane and furoeremophilane sesquiterpenoids | [M+H]+ | 235.1686 | 107.08533, 189.16304, 217.15884, 235.17001 | 0.0006564 |
| 14 | 15.12 | Unknown-2 | C15H26O3 | - | [M–H2O+H]+ | 237.1839 | 105.07021, 145.10126, 161.13174, 179.14192, 201.16489, 237.18439 | 0.0010065 |
| 15 | 14.91 | Unknown-3 | C15H24O2 | - | [M+H]+ | 237.1841 | 105.07066, 145.10062, 161.13272, 179.14333, 201.16388, 237.18645 | 0.0008065 |
| 16 | 14.56 | (1aS,10aR)-1a,5,9-Trimethyl-1a,3,6,10a-tetrahydrooxireno[4,5]cyclodeca[1,2-b]furan-10(2H)-one | C15H18O3 | Germacrane sesquiterpenoids | [M+H]+ | 247.132 | 123.08041, 139.0396, 229.15799, 247.20444 | 0.0008709 |
| 17 | 15.38 | Atractylenolide III | C15H20O3 | Eudesmanolides, secoeudesmanolides, and derivatives | [M+H]+ | 249.1476 | 105.06987, 163.11208, 190.93147, 231.13821, 249.18474 | 0.000921 |
| 18 | 11.57 | Naphtho[2,3-b]furan-2(4H)-one, 4a,5,6,7,8,8a,9,9a-octahydro-9,9a-dihydroxy-3,4a,5-trimethyl-, (4aR,5S)- | C15H22O4 | Terpene lactones | [M–H2O+H]+ | 249.1477 | 81.07021, 109.10094, 147.11635, 175.14827, 187.14833, 203.17921, 231.17542, 249.18481 | 0.000821 |
| 19 | 15.16 | 1(4H)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-6-hydroxy-4-(hydroxymethyl)-3,4a,8,8-tetramethyl- | C15H24O3 | Cyclohexenones | [M+H]+ | 253.1786 | 95.08618, 133.1015, 189.16336, 217.15929, 253.17986 | 0.0012211 |
| 20 | 10.15 | Aloe-emodin | C15H10O5 | Anthraquinones | [M+H]+ | 271.0597 | 68.10496, 153.01845, 251.16299, 271.06143 | 0.0003999 |
| 21 | 8.59 | 7,3',4'-Trihydroxyflavone | C15H10O5 | - | [M+H]+ | 271.0605 | 81.07014, 137.02362, 215.07114, 271.06143 | -0.0004001 |
| 22 | 20.11 | Galaxolidone | C18H24O2 | 2-benzopyrans | [M+H]+ | 273.1841 | 67.05447, 157.09996, 255.17398, 273.1871 | 0.0008065 |
| 23 | 20.43 | Norambreinolide | C16H26O2 | Naphthofurans | [M+Na]+ | 273.1844 | 68.4108157.10152, 255.17357, 273.1853 | -0.0018992 |
| 24 | 26.04 | 2-Penten-1-ol, 5-[(1S,4aS,8aS)-decahydro-5,5,8a-trimethyl-2-methylene-1-naphthalenyl]-3-methyl-, (2E)- | C20H34O | Diterpenoids | [M–H2O+H]+ | 273.2568 | 95.08594, 149.13184, 217.19507, 273.25818 | 0.0008775 |
| 25 | 14.04 | Piperine | C17H19NO3 | Alkaloids and derivatives | [M+H]+ | 286.143 | 67.99371, 135.04471, 201.05357, 240.23338, 286.29395 | 0.0007699 |
| 26 | 10.40 | Luteolin | C15H10O6 | Flavones | [M+H]+ | 287.0537 | 68.99779, 153.01805, 213.05312, 258.05023, 287.0531 | 0.0013145 |
| 27 | 7.90 | Kaempferol | C15H10O6 | Flavonols | [M+H]+ | 287.0549 | 68.66821, 151.07494, 210.37479, 259.06134, 264.87177, 287.05881 | 0.0001145 |
| 28 | 17.59 | 8-[3-oxo-2-[(E)-pent-2-enyl]cyclopenten-1-yl]octanoic acid | C18H28O3 | - | [M+H]+ | 293.2097 | 105.06985, 219.17538, 275.20047, 293.21146 | 0.0014212 |
| 29 | 18.32 | 2'-Methoxyformonetin | C17H14O5 | 4'-O-methylisoflavones | [M+H]+ | 299.09 | 68.17657, 256.07022, 299.09021 | 0.0014 |
| 30 | 17.41 | RETUSIN 7-METHYL ETHER | C17H14O5 | 7-O-methylisoflavones | [M+H]+ | 299.0909 | 81.07018, 256.07413, 299.09021 | 0.0005 |
| 31 | 21.59 | 7-[(2E)-3,7-dimethylocta-2,6-dienoxy]chromen-2-one | C19H22O3 | Terpene lactones | [M+H]+ | 299.163 | 81.07011, 163.03951, 245.22661, 299.25693 | 0.001171 |
| 32 | 10.40 | Fallacinol | C16H12O6 | Anthraquinone | [M+H]+ | 301.0699 | 81.07058, 119.08566, 258.05148, 301.07086 | 0.0007646 |
| 33 | 24.03 | Retinoic acid | C20H28O2 | Retinoids | [M+H]+ | 301.2152 | 81.07059, 123.11665, 159.11688, 209.13231, 259.1673, 301.21463 | 0.0010066 |
| 34 | 9.37 | Unknown-4 | C18H29NO3 | - | [M+H]+ | 308.222 | 107.08547, 192.13922, 308.22241 | 2.02E-05 |
| 35 | 13.76 | Bisdemethoxycurcumin | C19H16O4 | Curcuminoids | [M+H]+ | 309.1113 | 91.05478, 119.08567, 147.04324, 225.09119, 275.20135, 309.11188 | 0.0008354 |
| 36 | 1.29 | Unknown-5 | C15H19NO6 | - | [M+H]+ | 310.1279 | 69.07032, 120.08043, 166.08688, 244.09789, 264.12106, 310.12964 | 0.0006138 |
| 37 | 14.41 | (E)-4-[(1R,2S,3S,4R,8aS)-2,3,4-trihydroxy-2,5,5,8a-tetramethyl-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl]but-3-en-2-one | C18H30O4 | Sesquiterpenoids | [M+H]+ | 311.2212 | 81.0341, 105.07024, 275.20117, 311.2207 | 0.0004859 |
| 38 | 13.7 | Triptophenolide | C15H24N2O5 | Oxosteroids | [M+H]+ | 313.1764 | 68.80101, 95.0859, 268.2641, 313.31876 | -0.0006017 |
| 39 | 10.6 | Isorhamnetin | C16H12O7 | Flavonols | [M+H]+ | 317.0657 | 68.07446, 95.08575, 153.01782, 212.2003, 317.17227 | -0.0001208 |
| 40 | 16.68 | (S)-[6]gingerol | C17H26O4 | Gingerols | [M+Na]+ | 317.1705 | 68.88292, 231.63303, 317.17349 | 0.00183 |
| 41 | 22.76 | 1-Naphthalenecarboxylic acid, decahydro-5-[(3E)-5-hydroxy-3-(hydroxymethyl)-3-penten-1-yl]-1,4a-dimethyl-6-methylene- | C20H32O4 | Diterpenoids | [M–H2O+H]+ | 319.2254 | 57.86268, 109.10156, 217.1588, 273.18475, 319.2283 | 0.0013713 |
| 42 | 13.31 | 1-(4-hydroxy-3-methoxyphenyl)-6-methoxy-2,3-dimethyl-3,4-dihydro-1H-naphthalene-2,7-diol | C20H24O5 | Aryltetralin lignans | [M–H2O+H]+ | 327.1585 | 98.98486, 151.0746,174.9921, 250.99988, 289.47156, 327.2308 | 0.0005856 |
| 43 | 24.61 | Ceratodictyol | C19H38O4 | - | [M+H]+ | 331.2834 | 57.03428, 239.23659, 313.27094, 331.22485 | 0.0008861 |
| 44 | 23.38 | 5-[(8aS)-2,5,5,8a-tetramethyl-3-oxo-4a,6,7,8-tetrahydro-4H-naphthalen-1-yl]-3-methylpentanoic acid | C20H32O3 | Diterpenoids | [M+Na]+ | 343.2244 | 67.36462, 240.23369, 283.26526, 343.22202 | -3.44E-05 |
| 45 | 2.55 | (E)-3-[4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]prop-2-enoic acid | C15H18O8 | Phenolic glycosides | [M+NH4]+ | 344.1329 | 85.02883, 147.0433, 279.81799, 343.13223 | 0.0010931 |
| 46 | 24.76 | Darutigenol | C20H34O3 | Diterpenoids | [M+Na]+ | 345.2386 | 67.87338, 183.17409, 240.23366, 345.23901 | 0.0014156 |
| 47 | 7.71 | Citrusin | C16H22O7 | Phenolic glycosides | [M+Na]+ | 349.1263 | 97.02866, 123.11671, 257.14923, 349.19699 | -0.0005263 |
| 48 | 16.75 | Ingenol | C20H28O5 | Tigliane and ingenane diterpenoids | [M+H]+ | 349.1986 | 67.95583, 107.08621, 349.19705 | 0.0023504 |
| 49 | 5.58 | (2R,3R,4S,5S,6R)-2-[(2E)-4-hydroxy-3,7-dimethylocta-2,6-dienoxy]-6-(hydroxymethyl)oxane-3,4,5-triol | C16H28O7 | Terpene glycosides | [M+NH4]+ | 350.2156 | 67.9294, 93.06985, 107.08545, 135.11662, 153.12802, 176.00433 | 0.0017288 |
| 50 | 5.56 | 2-(hydroxymethyl)-6-(6-hydroxy-6-methyl-3-propan-2-ylcyclohex-3-en-1-yl)oxyoxane-3,4,5-triol | C16H28O7 | Terpene glycosides | [M+Na]+ | 355.1722 | 67.90975, 168.95718, 218.86839, 308.9007, 355.1712 | 0.0005239 |
| 51 | 18.54 | 14-Deoxyandrographolide | C20H30O4 | Diterpene lactones | [M+Na]+ | 357.2026 | 68.28679, 198.79074, 357.25626 | 0.0010301 |
| 52 | 18.54 | Unknown-6 | C23H41NO2 | - | [M+H]+ | 364.3202 | 67.05444, 93.06979, 305.24673, 364.32092 | 0.000806 |
| 53 | 14.47 | (1E,4Z,6E)-5-hydroxy-1,7-bis(4-hydroxy-3-methoxyphenyl)hepta-1,4,6-trien-3-one | C21H20O6 | Curcuminoids | [M+H]+ | 369.1326 | 89.03889, 117.03339, 145.02832, 177.0547, 219.06584, 245.08064, 285.11255, 369.12991 | 0.0006648 |
| 54 | 13.53 | Lagochilin | C20H36O5 | Diterpenoid | [M+Na]+ | 379.2452 | 68.24915, 95.5078, 174.91986, 379.24777 | 0.000295 |
| 55 | 29.84 | Dioctyl Phthalate | C24H38O4 | Benzoic acid esters | [M+H]+ | 391.2841 | 71.0862, 149.02263,167.03416, 279.16132 | 0.0001861 |
| 56 | 20.49 | gamma-mangostin | C23H24O6 | 8-prenylated xanthones | [M+H]+ | 397.1637 | 81.07045, 141.09119, 231.17474, 257.04388, 285.03897, 341.10275, 397.16495 | 0.0008649 |
| 57 | 1.27 | Riboflavin | C17H20N4O6 | Flavins | [M+Na]+ | 399.1264 | 67.76998, 121.55795, 321.87012, 399.12759 | 0.0011051 |
| 58 | 4.37 | 7-(4-hydroxyphenyl)-2,2,10,10-tetramethyl-11,12-dihydro-2H-dipyrano[2,3-f:2',3'-h]chromen-8(10H)-one | C23H24N4OS | 6-prenylated isoflavanones | [M+H]+ | 405.1717 | 67.69054, 133.10126, 161.26315, 405.16913 | 0.0026588 |
| 59 | 11.27 | (3aR,3a1S,5S,5aS,10bS)-methyl 6-acetyl-3a-ethyl-2,3,3a,3a1,4,5,5a,6,11,12-decahydro-1H-indolizino[8,1-cd]carbazole-5-carboxylate | C21H34O6 | Aspidospermatan-type alkaloids | [M+Na]+ | 405.2238 | 68.69836, 145.10095, 341.79178, 405.22348 | 0.0009595 |
| 60 | 3.94 | 3-Buten-2-one, 4-[4-(beta-D-glucopyranosyloxy)-2-hydroxy-2,6,6-trimethylcyclohexylidene]- | C19H30O8 | Terpene glycosides | [M+Na]+ | 409.1823 | 67.82968, 93.64545, 148.11446, 409.17404 | 0.0009886 |
| 61 | 27.16 | Lup-20(29)-en-3-ol, (3alpha)- | C30H50O | Triterpenoids | [M–H2O+H]+ | 409.3828 | 67.05487, 81.0707,95.04983, 109.10178, 137.13298, 191.18045, 231.21114, 372.78149, 409.38425 | 7.80E-05 |
| 62 | 22.47 | Cratoxyarborenone E | C24H26O6 | 4-prenylated xanthones | [M+H]+ | 411.1799 | 68.88006, 355.11905, 411.1813 | 0.000315 |
| 63 | 6.64 | 2-Butanone, 4-[3-(beta-D-glucopyranosyloxy)-4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl]- | C19H32O8 | Terpene glycosides | [M+Na]+ | 411.1989 | 67.38717, 205.50575, 411.19666 | 3.87E-05 |
| 64 | 29.84 | 2-acetoxy-4-pentadecylbenzoic acid | C24H38O4 | Acylsalicylic acids | [M+Na]+ | 413.2645 | 68.1461, 301.14127, 413.26453 | 0.0017304 |
| 65 | 15.55 | 2H-Oxireno[1,10a]phenanthro[3,2-b]furan-10(11bH)-one, 5,7-bis(acetyloxy)-3,3a,4,5,6,7,7a,7b,8,8a-decahydro-4,4,7a,11-tetramethyl-, (1aS,3aR,5S,7S,7aR,7bS,8aR,11bR)- | C24H32O7 | Naphthofurans | [M–H2O+H]+ | 415.2117 | 67.71227, 79.05482, 91.055, 107.08614, 119.0854, 135.08011 | -0.0001849 |
| 66 | 14.13 | 6-[3-[(3,4-dimethoxyphenyl)methyl]-4-methoxy-2-(methoxymethyl)butyl]-4-methoxy-1,3-benzodioxole | C24H32O7 | Dibenzylbutane lignans | [M–H2O+H]+ | 415.21 | 67.69196, 119.0854, 253.83365 | 0.0015151 |
| 67 | 7.76 | Cyanidin-3-O-alpha-arabinoside | C20H19O10 | Flavonoid-3-O-glycosides | [M]+ | 419.0958 | 57.07051, 133.10123, 213.05363, 287.05383, 289.06158 | 0.0014732 |
| 68 | 3.46 | 6,7-dimethyl-4-(((4-oxo-3-phenyl-4H-chromen-7-yl)oxy)methyl)-2H-chromen-2-one | C20H24O10 | Isoflavones | [M+H]+ | 425.1412 | 68.1309, 373.84241, 425.13763 | 0.0030234 |
| 69 | 21.18 | 3-Epilupeol | C30H50O | Triterpenoids | [M+H]+ | 427.3892 | 67.62643, 95.08592,222.0757, 324.3266,427.3833 | 0.0042427 |
| 70 | 15.07 | 7b,9-Dihydroxy-3-(hydroxymethyl)-1,1,6,8-tetramethyl-5-oxo-1,1a,1b,4,4a,5,7a,7b,8,9-decahydro-9aH-cyclopropa[3,4]benzo[1,2-e]azulen-9a-yl acetate | C22H30O6 | Tigliane and ingenane diterpenoids | [M+ACN+H]+ | 432.2369 | 69.07071, 119.08536, 281.13596, 415.21252, 431.27979 | 0.0011642 |
| 71 | 6.30 | isovitexin | C21H20O10 | Flavonoid C-glycosides | [M+H]+ | 433.1123 | 68.35822, 165.01753, 283.05933, 313.07135, 314.07736, 433.11243 | 0.0006233 |
| 72 | 8.91 | Cyanidin-3-O-rhamnoside | C21H21O10 | Anthocyanidin-3-O-glycosides | [M]+ | 433.1118 | 67.63067, 149.02264, 287.05307, 433.21448 | 0.0011233 |
| 73 | 7.11 | quercetin-3-O-pentoside | C20H18O11 | Flavonoid-3-O-glycosides | [M+H]+ | 435.0908 | 73.80537, 115.03951, 229.05016, 303.04858, 349.74323 | 0.0013878 |
| 74 | 7.33 | avicularin | C20H18O11 | Flavonoid-3-O-glycosides | [M+H]+ | 435.0927 | 67.65572, 149.0231, 215.43008, 304.05154 | -0.0005122 |
| 75 | 16.32 | Magnolin | C23H28O7 | Furanoid lignans | [M+Na]+ | 439.172 | 68.45914, 150.43907, 290.24887, 439.1684 | 0.0007239 |
| 76 | 28.6 | Betulin | C30H50O2 | Triterpenes | [M+H]+ | 443.3887 | 81.07026, 268.14828, 358.70224, 443.33624 | -0.0003427 |
| 77 | 14.8 | Benzenepropanamide, N-[2-(acetyloxy)-1-(phenylmethyl)ethyl]-alpha-(benzoylamino)- | C27H28N2O4 | Phenylalanine and derivatives | [M+H]+ | 445.211 | 105.03419, 194.11877, 224.10695, 252.10074, 380.17337, 398.18967 | 0.0011838 |
| 78 | 7.21 | Quercitrin | C21H20O11 | Flavonoid-3-O-glycosides | [M+H]+ | 449.1067 | 85.02866, 129.05505, 303.04739, 389.34125 | 0.0011379 |
| 79 | 1.09 | 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxychromen-4-one | C21H20O11 | Flavonoid-3-O-glycosides | [M+H]+ | 449.1082 | 71.04998, 129.05507, 229.04935, 303.05249, 449.19958 | -0.0003621 |
| 80 | 15.07 | 5-O-methylvisammioside | C24H24N2O7 | Furanochromones | [M+H]+ | 453.1659 | 67.65093, 293.21219, 453.16299 | -0.0002724 |
| 81 | 7.91 | Afzelin | C22H16N4O6 | Flavonoid-3-O-glycosides | [M+Na]+ | 455.094 | 67.6265, 107.08612, 169.04633, 309.03836, 455.20956 | 0.0022049 |
| 82 | 7.07 | Quercetin 3-O-alpha-L-Arabinopyranoside | C20H18O11 | Flavonoid-3-O-glycosides | [M+Na]+ | 457.0726 | 67.45666, 325.03085, 457.23947 | 0.0015321 |
| 83 | 7.52 | Peonidin-3-O-glucoside | C22H23O11 | Anthocyanidin-3-O-glycosides | [M]+ | 463.1242 | 68.18273, 301.07108, 463.12286 | -0.000712 |
| 84 | 8.49 | 2-[[3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxymethyl]-6-[(6,6-dimethyl-4-bicyclo[3.1.1]hept-3-enyl)methoxy]oxane-3,4,5-triol | C21H34O10 | Terpene glycosides | [M+NH4]+ | 464.248 | 81.07057, 196.15639, 303.05344, 463.1618 | 0.0010228 |
| 85 | 6.46 | Isoquercitrin | C21H20O12 | Flavonoid-3-O-glycosides | [M+H]+ | 465.1024 | 85.02865, 238.41808, 303.04709, 398.30258 | 0.0003525 |
| 86 | 1.41 | Hyperoside | C21H20O12 | Flavonoid-3-O-glycosides | [M+H]+ | 465.1042 | 68.23981, 245.83891, 303.05246, 429.02948 | -0.0014475 |
| 87 | 8.87 | (2R,3S,4S,5R,6R)-2-[[(2R,3R,4R,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]oxymethyl]-6-[(2E)-3,7-dimethylocta-2,6-dienoxy]oxane-3,4,5-triol | C21H36O10 | Terpene glycosides | [M+NH4]+ | 466.2646 | 81.07049, 137.13251, 303.04739, 420.24896 | 7.29E-05 |
| 88 | 6.93 | Homoorientin | C21H20O11 | Flavonoid C-glycosides | [M+Na]+ | 471.0895 | 67.58913, 243.48718, 325.03052, 471.08929 | 0.0002822 |
| 89 | 16.56 | (1R,3aS,5aR,5bR,11aR,13aR)-7-hydroxy-5a,5b,8,8,11a-pentamethyl-9-oxo-1-prop-1-en-2-yl-2,3,4,5,6,7,7a,10,11,11b,12,13,13a,13b-tetradecahydro-1H-cyclopenta[a]chrysene-3a-carboxylic acid | C30H46O4 | Triterpenoids | [M+H]+ | 471.346 | 81.07048, 362.94534, 470.36197 | 0.0008864 |
| 90 | 29.26 | Oleanolic acid | C30H48O3 | Triterpenoids | [M+Na]+ | 479.3476 | 67.54087, 158.6881, 274.99387, 435.37073, 479.35306 | 0.0019661 |
| 91 | 7.38 | beta-D-Glucopyranoside, (1R,2S,4R,5R)-5-hydroxy-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl 6-O-[(2R,3R,4R)-tetrahydro-3,4-dihydroxy-4-(hydroxymethyl)-2-furanyl]- | C21H36O11 | Terpene glycosides | [M+Na]+ | 487.2159 | 67.72539, 335.0957, 487.2117 | -0.0009173 |
| 92 | 27.66 | Glycyrrhetic acid | C30H46O4 | Triterpenoids | [M+Na]+ | 493.3274 | 68.00111, 259.16779, 493.32791 | 0.0014307 |
| 93 | 7.59 | Quercetin-3-O-glucosyl-6''-acetate | C23H22O13 | Flavonoid-3-O-glycosides | [M+H]+ | 507.1137 | 68.89761, 303.04816, 427.18243 | -0.0003828 |
| 94 | 7.46 | 3,4-di-O-caffeoylquinic acid | C25H24O12 | Quinic acids and derivatives | [M+H]+ | 517.1346 | 67.46111, 117.03333, 145.04965, 164.04106 | -0.0005473 |
| 95 | 24.63 | Ganoderic Acid A | C30H44O7 | Triterpenoids | [M+H]+ | 517.3115 | 67.96053, 296.56985, 395.65579, 517.31256 | 0.0044802 |
| 96 | 22.98 | Angeloylgomisin H | C27H36N2O5S | Hydrolyzable tannins | [M+Na]+ | 523.2252 | 67.48286, 144.31828, 382.56818, 523.24292 | -0.001486 |
| 97 | 27.29 | lappaconitine | C34H40N4O5 | Lappaconitine-type diterpenoid alkaloids | [M+Na]+ | 607.2898 | 67.0547, 95.08575, 303.04739, 344.08575 | -0.0007089 |
| 98 | 6.24 | Rutin | C27H30O16 | Flavonoid-3-O-glycosides | [M+H]+ | 611.1605 | 85.02868, 129.05518, 229.04927, 303.04742, 355.0686 | 0.0001613 |
| 99 | 5.51 | Quercetin-3-O-rutinoside | C27H30O16 | Flavonoid-3-O-glycosides | [M+H]+ | 611.1606 | 85.02868, 149.04514, 303.04758, 522.49298 | 6.13E-05 |
| 100 | 25.33 | (E)-6-((7-acetamido-1,2,3-trimethoxy-9-oxo-5,6,7,9-tetrahydrobenzo[a]heptalen-10-yl)amino)-N-(3,4,5,6-tetrahydro-2H-cyclopenta[d]thiazol-2-ylidene)hexanamide | C36H36N4O6 | Tropones | [M+H]+ | 621.2683 | 67.8502, 203.80643, 318.37054, 621.45972 | 0.0024613 |
| 101 | 6.96 | 5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-3-[3,4,5-trihydroxy-6-[[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxychromen-4-one | C28H32O16 | Flavonoid-3-O-glycosides | [M+H]+ | 625.1758 | 85.02876, 129.05522, 232.78003, 317.06549 | 0.0005114 |
| 102 | 10.34 | N1,N5,N10,N14-Tetra-trans-p-coumaroylspermine | C46H50N4O8 | Coumaric acids and derivatives | [M+H]+ | 787.3691 | 68.46892, 147.04326, 204.10252, 289.67331, 355.8197, 416.80713 | 0.001041 |

Negative mode

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No** | **RT (min)** | **Metabolite name** | **Formula** | **Ontology** | **Precursor type** | **Precursor mz** | **MS/MS spectrum** | **Mass error** |
| 1 | 1.08 | (1r,3R,4s,5S)-4-{[(2E)-3-(3,4-Dihydroxyphenyl)-2-propenoyl]oxy}-1,3,5-trihydroxycyclohexanecarboxylic acid | C16H18O9 | Quinic acids and derivatives | 353.08817 | [M–H]–  | 61.98749, 135.04468,191.05586, 315.07422,353.08667 | -0.0007943 |
| 2 | 1.09 | Rutoside (rutin) | C27H30O16 | Flavonoid-3-O-glycosides | 609.14508 | [M–H]– | 67.78544, 128.03394, 271.02518, 301.03833 | -0.0001633 |
| 3 | 1.10 | (1R,3R,4S,5R)-1,3,4-trihydroxy-5-[(E)-3-(4-hydroxyphenyl)prop-2-enoyl]oxycyclohexane-1-carboxylic acid | C16H18O8 | Quinic acids and derivatives | 337.0932 | [M–H]– | 61.98748, 119.04876, 163.03886, 337.09555 | -0.0003089 |
| 4 | 1.36 | Benzoic acid + 1O, 2MeO, O-Hex | C15H20O10 | Phenolic glycosides | 359.0993 | [M–H]– | 67.8550, 138.03183, 197.04433, 215.00694 | -0.0009296 |
| 5 | 1.56 | Hirsutrin | C21H20O12 | Flavonoid-3-O-glycosides | 463.08795 | [M–H]– | 67.91639, 151.00278, 300.02524, 463.08716 | 0 |
| 6 | 1.64 | Coumaroyl Hexoside | C15H18O8 | Coumaric acid and derivatives | 325.09299 | [M–H]– | 59.01262, 163.03897, 324.13983 | -0.0001943 |
| 7 | 2.36 | Chlorogenic acid | C16H18O9 | Quinic acids and derivatives | 353.0882 | [M–H]– | 67.57175, 191.05406, 293.03369 | -0.0003943 |
| 8 | 2.77 | Caffeoylquinic acid | C16H18O9 | Quinic acids and derivatives | 353.08817 | [M–H]– | 67.91013, 135.0450, 191.05623, 258.85776 | 0.000133 |
| 9 | 5.09 | Methyl chlorogenate | C17H20O9 | Quinic acids and derivatives | 367.1026 | [M–H]– | 67.84386, 173.04552, 361.79022 | 0.0007628 |
| 10 | 6.30 | Vitexin | C21H20O10 | Flavonoid 8-C-glycosides | 431.09763 | [M–H]– | 68.66195, 117.03347, 311.05511, 431.10284 | -0.0012649 |
| 11 | 6.45 | Hyperoside | C21H20O12 | Flavonoid-3-O-glycosides | 464.0954761 | [M–H]– | 67.64908, 300.0246,463.086, 781.51788 | -0.0011296 |
| 12 | 6.86 | Kaempferol-3-O-rutinoside | C27H30O15 | Flavonoid-3-O-glycosides | 593.15131 | [M–H]– | 67.65766, 97.04917, 285.04144 | -7.97E-05 |
| 13 | 6.92 | Avicularin | C20H18O11 | Flavonoids | 433.07788 | [M–H]– | 67.91952, 172.1398, 300.02939, 433.0788 | -0.0002651 |
| 14 | 7.00 | Kaempferol 3-alpha-L-arabinopyranoside | C20H18O10 | Flavonoid-3-O-glycosides | 417.08182 | [2M–H]– | 67.41055, 285.04016, 375.14221, 417.08295 | 0.0004121 |
| 15 | 7.43 | Kaempferol-3-O-alpha-L-arabinoside | C20H18O10 | Flavonoid-3-O-glycosides | 417.08368 | [M–H]– | 67.47419, 255.02872, 417.08127 | -0.0003313 |
| 16 | 7.76 | Kaempferol-3-O-arabinoside | C20H18O10 | Flavonoid-3-O-glycosides | 417.08194 | [M–H]– | 67.61118, 285.04114, 417.08197 | -0.0011737 |
| 17 | 8.58 | 7,3',4'-Trihydroxyflavone | C15H10O5 | Flavones | 269.046 | [M–H]– | 59.0126, 133.02867, 269.17331 | -0.000453 |
| 18 | 8.91 | Eriodictyol | C15H12O6 | Flavanones | 287.05643 | [M–H]– | 68.55089, 107.01304, 151.00253, 183.91185, 239.90402, 287.05551 | 0.0006894 |
| 19 | 9.08 | 3',4',5,7-tetrahydroxyflavone | C15H10O6 | Flavonoids | 285.0402 | [M–H]– | 67.62815, 241.05057, 285.04187 | 0.0002616 |
| 20 | 9.11 | 4-[(E)-2-(3-Hydroxy-5-methoxyphenyl)vinyl]phenyl beta-D-glucopyranoside | C21H24O8 | Stilbene glycosides | 403.14008 | [M–H]– | 67.87389, 241.08493, 293.00433 | 0.0008558 |
| 21 | 9.16 | Quercetin | C15H10O7 | Flavonols | 301.03494 | [M–H]– | 65.00222, 107.01268, 151.00307, 178.99861, 273.03909, 301.20316 | 0.0005538 |
| 22 | 9.29 | Rubiadin | C15H10O4 | Phenols | 253.0507 | [M–H]– | 68.42798, 121.0652, 191.14439, 225.05457, 253.14409 | 6.80E-05 |
| 23 | 9.40 | Unknown-1 | C13H16O8 | - | 299.0778 | [M–H]– | 97.04988, 158.95903, 205.08658 | -0.000559 |
| 24 | 9.90 | Unknown-2 | C13H16O9 | - | 315.0722 | [M–H]– | 83.04852, 125.09594, 225.11226 | -4.44E-05 |
| 25 | 10.15 | Apigenin | C15H10O5 | Flavones | 269.0452 | [M–H]– | 68.56183, 117.03371, 205.15955, 269.17346 | 0.000347 |
| 26 | 10.39 | Luteolin | C15H10O6 | Flavones | 285.04053 | [M–H]– | 68.63261, 151.0023, 229.05145, 285.04108 | -0.0008797 |
| 27 | 10.40 | Chrysoeriol | C16H12O6 | 3'-O-methylated flavonoids | 299.05579 | [M–H]– | 68.01218, 151.00273, 299.05737 | -0.0014385 |
| 28 | 10.60 | Isorhamnetin | C16H12O7 | Flavonols | 315.05225 | [M–H]– | 67.62162, 151.0023, 315.0528 | -0.0005106 |
| 29 | 11.08 | (4aR,5S)-9,9a-dihydroxy-3,4a,5-trimethyl-5,6,7,8,8a,9-hexahydro-4H-benzo[f][1]benzofuran-2-one | C15H22O4 | Terpene lactones | 265.1455 | [M–H]– | 67.69959, 96.9595,128.1839, 177.12747, 265.1467 | -0.0009673 |
| 30 | 11.89 | Unknown-3 | C12H14O3 | - | 205.0867 | [M–H]– | 99.92427, 135.04366, 158.97646, 271.15695 | 0.0003179 |
| 31 | 12.52 | (1S,8R,9R)-8-hydroxy-4-(propan-2-ylidene)-10-oxatricyclo[7.2.1.01,5]dodecane-8-carboxylic acid | C15H22O4 | Alpha hydroxy acids and derivatives | 265.1421 | [M–H]– | 67.35619, 96.95885, 135.7607, 197.15202, 265.14359 | 0.0024327 |
| 32 | 13.42 | 2-[(2S,4aR,8aS)-2-hydroxy-4a-methyl-8-methylidene-3,4,5,6,7,8a-hexahydro-1H-naphthalen-2-yl]prop-2-enoic acid | C15H22O3 | Eudesmane, isoeudesmane or cycloeudesmane sesquiterpenoids | 249.15 | [M–H]– | 68.16764, 112.9850, 180.89803, 205.15875, 249.14977 | -0.0003819 |
| 33 | 14.46 | (1E,4Z,6E)-5-hydroxy-1,7-bis(4-hydroxy-3-methoxyphenyl)hepta-1,4,6-trien-3-one | C21H20O6 | Curcuminoids | 367.1192 | [M–H]– | 68.04308, 134.03581, 217.04843, 298.15714, 367.16199 | -0.0004881 |
| 34 | 15.77 | Emodin | C15H10O5 | Hydroxyanthraquinones | 269.04544 | [M–H]– | 68.21111, 181.06483, 225.05499, 269.04395 | 0.0004039 |
| 35 | 16.55 | Unknown-4 | C12H18O4 | - | 225.1133 | [M–H]– | 97.05656, 181.89726, 224.20872, 267.19516, 285.20584 | -6.74E-05 |
| 36 | 16.89 | 9,12,15-Octadecatrienoic acid, 3-(hexopyranosyloxy)-2-hydroxypropyl ester, (9Z,12Z,15Z)- | C27H46O9 | Glycosylmonoacylglycerols | 559.31165 | [M–H]– | 67.56149, 97.04895, 253.09351, 277.21786, 278.22379 | 0.0006814 |
| 37 | 18.00 | Dinoseb | C10H12N2O5 | Dinitrophenols | 239.06737 | [M–H]– | 68.0143, 150.91476, 207.03963, 239.06795 | -0.0001089 |
| 38 | 18.39 | (E)-5-(2,3-dimethyl-4,5,6,7-tetrahydro-1H-tricyclo[2.2.1.02,6]heptan-3-yl)-2-methylpent-2-enoic acid | C15H22O2 | Sesquiterpenoids | 233.1546 | [M–H]– | 68.65767, 99.92443, 187.94162, 233.1534 | 0.0001035 |
| 39 | 18.57 | Unknown-5 | C15H12O5 | - | 271.0611 | [M–H]– | 67.56375, 174.95667, 289.17923 | 9.70E-05 |
| 40 | 20.44 | (E)-5-(1,2,4a,5-tetramethyl-7-oxo-3,4,8,8a-tetrahydro-2H-naphthalen-1-yl)-3-methylpent-2-enoic acid | C20H30O3 | Colensane and clerodane diterpenoids | 317.2115 | [M–H]– | 68.06743, 112.98454, 145.2968, 273.22205, 317.21216 | 0.0007184 |
| 41 | 21.55 | 5-[5-(acetyloxymethyl)-1,2,4a-trimethyl-7-oxo-3,4,8,8a-tetrahydro-2H-naphthalen-1-yl]-3-methylpentanoic acid | C22H34O5 | Diterpenoid | 377.2361 | [M–H]– | 79.95642, 311.16971, 377.23874 | -0.0027523 |
| 42 | 22.47 | Cratoxyarborenone E | C24H26O6 |  | 409.16528 | [M–H]– | 68.05138, 152.99466, 351.08737, 409.27618 | -0.0005883 |
| 43 | 23.46 | Aurapten | C19H22O3 | Terpene lactones | 297.1529 | [M–H]– | 67.74747, 119.049, 183.01189, 297.1535 | 8.92E-05 |
| 44 | 24.04 | 6,8-dihydroxy-2,2,4,4-tetramethyl-7-(3-methylbutanoyl)-9-(2-methylpropyl)-9H-xanthene-1,3-dione | C26H34O6 | Xanthenes | 441.2281 | [M–H]– | 56.77115, 148.02956, 255.7543, 369.13223, 441.22916 | 0.0001624 |
| 45 | 29.84 | Triptophenolide | C20H24O3 | Oxosteroids | 311.16806 | [M–H]– | 68.09985, 183.01161, 311.16971 | -6.77E-05 |