Supplementary Information



**Figure S1**. Selection of the stationary phase for the ultra-high performance liquid chromatography (UHPLC) separation of multicomponent from SHD. The total ion current (TIC) chromatograms are obtained in the positive high-definition MS mode.

**Table S6** Detailed information of the 236 components characterized from the SHD.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No. | RT (min) | Formula | Detected Mass (m/z) Ion Type | Error (ppm) | CCS (Å2) | MS/MS Fragments | Identification | Source |
| 1 | 2.10 | C6H8O7 | 191.0196[M–H]– | –0.50 | 262.48 | 173.0091,129.0193,111.0086,87.0086 | Citric acid | ASR,C,PRA |
| 2 | 2.15 | C16H24O10 | 421.1353[M–H]– | 0.20 | 188.80 | 375.1291,177.0563,165.0558 | 8-Epiloganic acid | RR |
| 3\* | 2.22 | C15H22O10 | 407.1194[M+HCOO]– | –0.3 | 186.68 | 361.1138,179.0558,161.0454,150.0420 | Catalpol | RR |
| 4 | 2.27 | C5H13N5O4 | 268.1044[M+H]+ | 1.60 | 262.15 | 136.0620,119.0351 | Adenosine | ASR |
| 5\* | 2.33 | C10H12N5O7P | 346.0550[M+H]+ | 1.00 | 182.08 | 152.0571,135.0305,110.0349 | Cyclic AMP | JF |
| 6 | 2.35 | C10H13N5O5 | 282.0844[M–H]– | –0.10 | 159.30 | 150.0420,133.0156,108.0195 | Guanosine | ASR |
| 7\* | 2.63 | C7H6O5 | 171.0291[M+H]+ | 1.60 | 187.94 | 153.0184,127.0391 | Gallic acid | ASR,C |
| 8\* | 2.69 | C27H42O20 | 709.2177[M+Na]+ | 2.10 | 237.23 | 687.2367,313.0896,147.0444 | Rehmannioside D | RR |
| 9 | 2.72 | C17H26O11 | 405.1390[M–H]– | –3.00 | 189.04 | 359.1338,295.1013,271.0453,259.0820,197.0816 | Morroniside | RR |
| 10 | 2.81 | C19H26O15 | 493.1189[M–H]– | –1.80 | 199.48 | 341.1069,313.0562,283.0443,169.0140,125.0244 | Galloylsucrose | GRR |
| 11\* | 2.86 | C21H32O15 | 523.1664[M–H]– | –0.80 | 214.90 | 507.1766,343.0988,181.0501,179.0554 | Melittoside | RR |
| 12 | 2.91 | C19H26O15 | 493.1197[M–H]– | –0.40 | 200.59 | 331.0671,313.0559,169.0139 | Diglucosyl gallic acid | GRR |
| 13 | 2.99 | C9H11NO2 | 166.0864[M+H]+ | 1.00 | 174.77 | 120.0812,103.0541,91.0541,77.0383 | L-Phenylalanine | ASR |
| 14 | 3.68 | C14H17N5O8 | 384.1152[M+H]+ | 0.40 | 188.45 | 252.0728,234.0628,188.0575,162.0778,136.0625 | Succinoadenosine | AR |
| 15\* | 4.76 | C11H12N2O2 | 205.0975[M+H]+ | 1.60 | 223.68 | 188.0707,170.0602,143.0730,130.0655,118.0652 | Tryptophan | ASR |
| 16 | 4.93 | C27H22O18 | 633.0730[M–H]– | –0.50 | 230.97 | 481.0623,331.0652,300.9984,275.0177 | Strictinin | PRA |
| 17 | 5.03 | C16H24O10 | 375.1289[M–H]– | –2.00 | 185.51 | 213.0772,169.0858,151.0764 | Desbenzoylpaeoniflorin | PRA |
| 18 | 6.12 | C30H26O12 | 579.1502[M+H]+ | 0.80 | 226.64 | 427.1042,409.0925,301.0724,287.0556,271.0609,247.0611 | Procyanidin B2 or its isomer | CR |
| 19 | 6.38 | C23H28O13S | 543.1171[M–H]– | –1.30 |  | 515.1415,375.0695,323.0762,179.0552 | Paeoniflorin sulfonate | PRA |
| 20 | 6.58 | C20H30O8 | 443.1922[M–H]– | –0.10 |  | 333.0982,303.1207,281.0660 | Cinncassiol E | CR |
| 21 | 6.62 | C23H28O12 | 519.1493[M+Na]+ | 4.00 |  | 497.1676,197.0823,179.0646,161.0598,121.0283 | Hydroxy-paeoniflorin | PRA |
| 22 | 6.84 | C30H26O12 | 579.1505[M+H]+ | 1.40 | 225.77 | 427.1063,409.0923,301.0723,287.0555,247.0611 | Procyanidin B2 or its isomer | CR |
| 23 | 7.16 | C16H26O8 | 369.1519[M+Na]+ | –0.10 | 190.21 | 347.1713,331.1288,319.1399,261.1260 | Rehmapicroside | RR |
| 24\* | 7.47 | C15H14O6 | 291.0863[M+H]+ | 0.10 | 163.14 | 245.0453,147.0443,139.0390,123.0442 | Catechin | CR,PRA |
| 25\* | 7.55 | C16H18O9 | 377.0843[M+Na]+ | 0.00 | 176.25 | 163.0392,145.0282,135.0443 | Chlorogenic acid | ASR,GRR |
| 26\* | 7.61 | C23H28O12 | 519.1472[M+Na]+ | –0.20 | 205.15 | 497.1652,179.0705,147.0446 | Oxypaeoniflorin | PRA |
| 27 | 7.86 | C19H28O11 | 431.1556[M–H]– | 0.60 | 203.88 | 477.1616,269.1026,161.0455 | Zizybeoside I | JF |
| 28 | 8.05 | C30H26O12 | 579.1503[M+H]+ | 1.00 | 228.83 | 427.1055,409.0927,301.0716,287.0552,271.0609,247.0610 | Procyanidin B2 or its isomer | CR |
| 29 | 8.16 | C27H24O18 | 635.0900[M–H]– | 1.60 | 234.07 | 483.0780,465.0683,421.0771,313.0556,295.0462,169.0143 | 3,4,6-Tetra-O-Galloyl-β-D-Glucose | PRA |
| 30 | 8.36 | C16H18O9 | 353.0876[M–H]– | –0.60 | 182.90 | 191.0560,179.0348,173.0454,161.0238,135.0451 | Cryptochlorogenic acid | ASR,GRR |
| 31\* | 8.61 | C9H8O4 | 181.0496[M+H]+ | 0.50 | 186.40 | 163.0391,145.0290,135.0443 | Caffeic acid | ASR |
| 32 | 8.84 | C25H38O16 | 593.2079[M–H]– | –1.3 | 239.87 | 639.2144,431.1559,413.1439,269.1027,161.0453 | Zizybeoside II | JF |
| 33 | 9.14 | C24H30O13 | 525.1620[M–H]– | –0.2 | 206.82 | 583.1187,511.1461,363.1078,327.1084,167.0350 | Mudanpioside E | PRA |
| 34 | 9.43 | C30H26O12 | 579.1496[M+H]+ | –0.10 | 231.20 | 441.1119,427.1027,409.0919,287.0558,271.0604,247.0604 | Procyanidin B2 or its isomer | CR |
| 35 | 9.46 | C18H26O10 | 401.1452[M–H]– | –0.40 | 201.05 | 447.1506,203.0708,161.0452 | Acetylcatalpol | RR |
| 36 | 9.61 | C29H38O16 | 687.2148[M+HCOO]– | 0.80 | 240.60 | 677.1869,641.2071,519.1722,475.1786,459.1862 | 6-O-β-D-Glucopyranosylalbiflorin | PRA |
| 37 | 9.82 | C27H32O14 | 579.1721[M–H]– | 0.30 | 228.30 | 417.1188,255.0661,135.0085 | Naringin | GRR |
| 38 | 9.90 | C27H24O18 | 635.0887[M–H]– | –0.50 | 226.72 | 483.0778,313.0535,169.0138 | 1,3,6-Tetra-O-Galloyl-β-D-Glucose | PRA |
| 39 | 9.92 | C18H19NO3 | 298.1437[M+H]+ | –0.10 | 174.56 | 269.1234,254.0935,238.0987,223.0766,192.1019,146.0604 | Stepharine | JF |
| 40 | 10.47 | C31H50O18 | 709.2932[M–H]– | 1.10 | 270.62 | 755.2978,547.2400,385.1855,319.1552,179.0557 | Zizvoside II | JF |
| 41\* | 10.70 | C15H14O6 | 289.0713[M–H]– | –1.50 | 167.36 | 271.0602,179.0345,151.0396,137.0243,109.0292 | L-Epicatechin | CR,PRA |
| 42 | 10.81 | C32H40O18 | 711.2141[M–H]– | –0.20 | 248.68 | 549.1616,255.0661 | Glucoliquiritin apioside | GRR |
| 43 | 10.97 | C29H38O16 | 687.2142[M+HCOO]– | 0.00 | 240.49 | 677.1836,641.2081,611.1990,593.1854,489.1615,471.1507,179.0555,121.0294 | 6-O-β-D-Glucosepaeoniflorin | PRA |
| 44\* | 11.16 | C23H28O11 | 503.1529[M+Na]+ | 1.10 | 212.99 | 481.1708,319.1179,301.1076,197.0811,179.0704,161.0600,151.0756,105.0335 | Albiflorin | PRA |
| 45 | 11.44 | C22H30O14 | 517.1555[M–H]– | –1.50 | 220.24 | 563.1613,355.1011,337.0611,193.0506,175.0403 | 6'-O-Feruloylsucrose | RR |
| 46 | 11.72 | C29H38O16 | 687.2146[M+HCOO]– | 0.60 | 245.19 | 641.2068,611.1978,519.1750,121.0275 | Isomaltosepaeoniflorin/β-gentiobiosyl paeoniflorin | PRA |
| 47\* | 11.80 | C25H24O12 | 515.1213[M–H]– | 3.50 | 212.17 | 353.0875,335.0757,191.0561,179.0346,135.0450 | 1,3-Dicaffeoylquinic acid | ASR,C |
| 48 | 11.91 | C29H38O16 | 687.2142[M+HCOO]– | 0.00 | 247.00 | 641.2068,611.1978,519.1749,489.1596,121.0275 | Isomaltosepaeoniflorin/β-gentiobiosyl paeoniflorin | PRA |
| 49 | 11.97 | C27H30O15 | 593.1507[M–H]– | –0.80 | 237.57 | 503.1178,473.1088,3830763,353.0662 | Vicenin-2 | GRR |
| 50 | 12.08 | C45H36O18 | 865.1983[M+H]+ | 1.00 | 286.80 | 713.1515,695.1412,533.1082,287.05512 | Cinnamtannin B1 | CR |
| 51\* | 12.39 | C45H38O18 | 867.2148[M+H]+ | 1.90 | 279.46 | 715.1662,579.1490,409.0914,301.0699,289.0663 | Procyanidin C1 | CR |
| 52\* | 12.43 | C23H28O11 | 481.1701[M+H]+ | 0.40 | 215.90 | 503.1526,197.0823,179.0714,151.0752,133.0656 | Peaoniflorin | PRA |
| 53 | 13.12 | C20H32O7 | 407.2051[M+H]+ | 2.70 | 179.69 | 349.2021,331.1919,313.1816,307.1170 | Cinnzeylanol | CR |
| 54 | 13.55 | C35H46O20 | 785.2494[M–H]– | –2.00 | 252.82 | 623.2186,451.1026,161.0239 | Purpureaside C | RR |
| 55 | 13.89 | C19H34O8 | 413.2151[M+Na]+ | 1.10 |  | 309.1401,193.1601,177.0922 | Rehmaionoside B its isomer | RR |
| 56\* | 14.13 | C26H28O14 | 563.1401[M–H]– | –0.90 | 230.91 | 545.1272,503.1200,473.1080,443.0980,383.0764,353.0656 | Schaftoside | GRR |
| 57 | 14.20 | C10H8O3 | 177.0546[M+H]+ | 0.00 | 183.07 | 162.0308,145.0286,134.0364,105.0335 | 7-Methoxycoumarin | GRR |
| 58\* | 14.29 | C10H10O4 | 195.0657[M+H]+ | 0.60 | 167.54 | 177.0553,149.0601,145.0289,134.0364,105.0331 | Ferulic acid | ASR,C |
| 59 | 14.72 | C17H17NO2 | 268.1337[M+H]+ | 1.80 |  | 251.1079,236.0842,219.0809,208.0892,191.0858,165.0716 | Asimilobine | JF |
| 60 | 14.76 | C30H24O12 | 577.1344[M+H]+ | 0.60 | 239.55 | 425.0884,299.0559,287.0552 | Proanthocyanidin A2 | CR |
| 61 | 14.93 | C21H22O10 | 457.1130[M+Na]+ | 1.70 | 161.60 | 435.1304,273.0765,255.0658 | Choerospondin | GRR |
| 62 | 14.94 | C21H22O10 | 433.1137[M–H]– | –0.80 | 205.83 | 313.0585,271.0611,253.0507,177.0192,151.0034,119.0491 | Isosalipurposide or its isomer | PRA |
| 63 | 14.99 | C41H30O26 | 937.0943[M–H]– | –1.10 | 296.57 | 767.0746,465.0653,313.0568,300.9990,265.0714,169.0140 | Eugeniin | GRR |
| 64 | 15.07 | C45H36O18 | 865.1963[M+H]+ | –1.30 | 286.09 | 713.1482,695.1400,533.1080,409.0929,287.0545 | Cinnamtannin D | CR |
| 65 | 15.26 | C34H28O22 | 789.1171[M+H]+ | 3.30 | 277.53 | 811.0983,771.1051,619.0961,449.0709,431.0605,261.0375,153.0184,125.0236 | 1,2,3,6-Tetra-O-Galloyl-β-D-Glucose | PRA |
| 66\* | 15.32 | C21H22O9 | 417.1184[M-H]- | –1.80 | 190.14 | 255.0659,135.0083 | Isoliquiritin | GRR |
| 67 | 15.55 | C23H28O13 | 525.1606[M+HCOO]– | –1.50 | 212.03 | 357.1168,121.0296 | Mudanpioside I | PRA |
| 68 | 15.64 | C26H30O13 | 549.1604[M–H]– | –1.80 | 212.17 | 429.1044,415.1014,399.1078 | Licuraside | GRR |
| 69 | 15.68 | C36H48O20 | 799.2653[M–H]– | –1.70 | 270.57 | 623.2185,605.2078,513.1605,293.0879,285.0403 | Jionoside A1 | JF |
| 70\* | 15.74 | C21H22O9 | 441.1160[M+H]+ | 1.00 | 191.92 | 419.1343,257.0811,137.0236 | Liquiritin | GRR |
| 71\* | 15.79 | C22H22O10 | 447.1289[M+H]+ | 0.70 | 213.76 | 285.0760,270.0524,253.0496 | Calycosin-7-O-β-D-glucoside | GRR,AR |
| 72 | 15.80 | C21H22O10 | 433.1136[M–H]– | –1.10 | 203.61 | 313.0553,271.0608,177.0190,151.0036,119.0501 | Isosalipurposide or its isomer | PRA |
| 73 | 15.86 | C19H34O8 | 413.2149[M+Na]+ | 0.80 |  | 319.1659,309.1383,161.0964 | Rehmaionoside B | RR |
| 74 | 15.87 | C34H28O22 | 787.0996[M–H]– | –0.50 | 268.67 | 635.0895,617.0786,465.0664,313.0567 | 1,2,3,6-Tetra-O-Galloyl-β-D-Glucose its isomer | PRA |
| 75 | 15.94 | C20H28O10 | 473.1667[M+HCOO]– | 0.40 | 212.86 | 427.1608,293.0867 | Rosavin | CR |
| 76 | 16.07 | C24H44N4O4 | 453.3448[M+H]+ | –2.90 |  | 475.3269,435.344,257.0824,137.0242 | Cyclo tetraleucyl | ASR |
| 77 | 16.12 | C14H6O8 | 303.0139[M+H]+ | 1.40 | 158.52 | 285.0046,257.0086 | Ellagic acid | PRA |
| 78 | 16.38 | C12H16O3 | 209.1173[M+H]+ | 0.30 |  | 191.1069,167.0731,163.1121,153.0547,121.0650,77.0384 | Senkyunolide G | C |
| 79\* | 16.66 | C27H30O14 | 577.1562[M–H]– | –0.10 | 236.71 | 623.1618,559.1442,457.1134,413.0877,383.0767,353.0662 | Violanthin | GRR |
| 80 | 16.84 | C25H40O12 | 577.2499[M+HCOO]– | –0.40 | 238.99 | 531.2442,463.2184,449.2027,354.1344 | Zizvoside I | JF |
| 81\* | 17.05 | C30H32O15 | 631.1658[M–H]– | –1.60 | 224.75 | 613.1563,509.1297,491.1191,399.0927,313.0558 | Galloylpaeoniflorin | PRA |
| 82 | 17.62 | C30H55N5O5 | 566.4296[M+H]+ | 3.50 |  | 588.4118,548.4168,453.3476,435.3336 | Cyclo pentaleucyl | ASR |
| 83\* | 17.88 | C29H36O15 | 623.1974[M–H]– | 1.20 | 225.60 | 461.1669,161.0248 | Verbascoside | RR |
| 84 | 18.20 | C30H32O15 | 631.1665[M–H]– | –0.50 |  | 613.1545,399.0927,313.0560,169.0136 | Galloylpaeoniflorin its isomer | PRA |
| 85\* | 18.53 | C41H32O26 | 963.1082[M+H]+ | 0.80 | 296.23 | 771.1044,619.0929,431.0614,261.0391,153.0184,125.0235 | Pentagalloyl glucose | PRA |
| 86 | 18.58 | C25H24O12 | 515.1210[M–H]– | 2.90 | 214.7 | 353.0869,335.0771,191.0561,179.0354,135.0446 | 3,5-Dicaffeoylquinic acid its isomer | ASR,C |
| 87 | 18.71 | C37H50O20 | 813.2816[M–H]– | –0.9 | 272.23 | 639.1936,637.2295,619.2223,175.0397 | Jionoside B1 | RR |
| 88 | 18.74 | C30H32O15 | 631.1664[M–H]– | –0.70 |  | 509.1277,399.0935,313.0560,169.0139,121.0292 | Galloylpaeoniflorin its isomer | PRA |
| 89\* | 18.93 | C25H24O12 | 515.1193[M–H]– | –0.40 | 210.29 | 353.0878,335.0771,191.0561,179.0350,135.0454 | 3,5-Dicaffeoylquinic acid | ASR,C |
| 90\* | 19.20 | C29H36O15 | 623.1974[M–H]– | 1.10 | 224.76 | 461.1669,161.0248 | Isoacteoside | RR |
| 91 | 19.45 | C21H22O10 | 433.1137[M–H]– | –0.60 | 184.18 | 271.0608,177.0194,151.0036 | 5,7-Dihydroxyflavanone-4'-O-β-D-glucoside | AR |
| 92 | 19.66 | C30H32O15 | 633.1818[M+H]+ | 1.60 | 236.03 | 471.1317,355.0738,301.1074,153.0182 | 4-O-Galloylalbiflorin | PRA |
| 93 | 19.74 | C12H16O4 | 247.0948[M+Na]+ | 2.70 | 147.88 | 207.1022,189.0918,161.0968,133.0656,91.0545 | Senkyunolide I | ASR,C |
| 94 | 20.07 | C36H66N6O6 | 679.5136[M+H]+ | 2.90 |  | 701.4937,453.3476,435.3336 | Cyclo senaryleucyl | ASR |
| 95 | 20.26 | C24H30O12 | 509.1667[M–H]– | 0.40 | 214.15 | 301.0701,179.0709 | Mudanpioside D | PRA |
| 96 | 20.36 | C23H28O11 | 479.1558[M–H]– | 0.30 | 216.92 | 525.1615,449.1426,357.1186,283.0816,195.0662,121.0294 | Albiflorin R1 | PRA |
| 97 | 20.73 | C25H24O12 | 515.1193[M–H]– | –0.40 | 213.86 | 353.0879,335.0772,191.0560,179.0349,135.0450 | 3,5-Dicaffeoylquinic acid its isomer | ASR,C |
| 98 | 20.87 | C30H38O15 | 637.2136[M–H]– | –0.30 | 245.41 | 461.1658,160.0164 | Leucoscceptoside A | RR |
| 99\* | 21.19 | C12H16O4 | 247.0948[M+Na]+ | 2.90 | 148.22 | 207.1023,189.0917,161.0968,133.0649,91.05380 | Senkyunolide H | ASR,C |
| 100 | 21.26 | C22H34O8 | 425.2178[M–H]– | –0.80 | 188.84 | 471.2237,383.2070,365.1963,329.1758,279.1237,261.1133 | Cinnzeylanine | CR |
| 101 | 21.27 | C23H26O10 | 507.1510[M–H]– | 0.40 | 212.13 | 461.1452,433.1505,373.1282,266.1142,177.0557,121.0290 | Lactiflorin | PRA |
| 102\* | 21.42 | C18H19NO2 | 282.1490[M+H]+ | 0.50 | 169.60 | 250.0991,235.0756,219.0804,191.0853,179.0856 | Ortho-nornuciferine | JF |
| 103\* | 22.24 | C26H30O13 | 551.1756[M+H]+ | –0.50 | 220.46 | 419.1375,257.0808,239.0698 | Isoliquiritin apioside | GRR |
| 104\* | 22.32 | C22H22O9 | 431.1336[M+H]+ | –0.10 | 209.26 | 453.1155,269.0808,254.0566,237.0546 | Ononin | AR,GRR |
| 105 | 22.67 | C15H10O4 | 255.0653[M+H]+ | 0.50 | 154.04 | 277.0485,213.0561,145.0288 | Chrysin | GRR |
| 106 | 22.78 | C21H22O9 | 419.1334[M+H]+ | –0.60 | 217.11 | 257.0809,239.0705,147.0447,137.0242 | Iiquiritin its isomer | GRR |
| 107 | 22.98 | C23H24O10 | 461.1450[M+H]+ | 1.60 | 218.17 | 299.0915,257.0812,239.0717 | 6''-O-Acetylliquiritin | GRR |
| 108 | 23.00 | C26H30O13 | 551.1769[M+H]+ | 1.70 | 238.30 | 573.1602,419.1337,257.0809 | Isoliquiritin apioside its isomer | GRR |
| 109 | 23.33 | C30H32O14 | 615.1717[M–H]– | –0.40 | 234.67 | 493.1349,475.1237,313.0562 | Mudanpioside H | PRA |
| 110 | 23.34 | C15H10O4 | 255.0654[M+H]+ | 0.90 | 152.74 | 277.0474,237.0549,137.0235,119.0493 | 4',7-Dihydroxyflavone | AR |
| 111\* | 23.50 | C15H12O4 | 257.0810[M+H]+ | 0.70 | 159.31 | 239.0712,147.0444,137.0236,119.0493 | Liquiritigenin | GRR |
| 112\* | 23.61 | C16H14O5 | 285.0766[M–H]– | –0.90 | 158.36 | 270.0526 | Licochalcone B | GRR |
| 113 | 23.72 | C21H22O5 | 355.1546[M+H]+ | 1.70 |  | 246.1291,215.1071,179.0699,177.1280,151.0396 | Licoagrochalcone C | GRR |
| 114 | 24.42 | C16H12O5 | 285.07575[M+H]+ | 0.00 | 163.06 | 270.0524,253.0501,161.0599,137.0232 | 7,8-Dihydroxy-4'-Methoxyisoflavone | AR |
| 115\* | 24.49 | C23H26O10 | 485.1434[M+Na]+ | 3.20 | 212.30 | 301.1074,269.0814,177.0551 | Methylnissolin-3-O-glucoside | AR |
| 116 | 24.61 | C35H36O15 | 695.1977[M–H]– | –0.60 | 249.29 | 549.1610,531.1509,417.1167,399.1076,277.0473,255.0657 | Licorice glycoside C1 | GRR |
| 117 | 24.72 | C21H34O10 | 445.208[M–H]– | 0.10 | 217.29 | 293.0874,233.0684,149.0448 | Pinen-10-yl-ß-vicianoside | PRA |
| 118 | 24.82 | C31H40O15 | 651.2297[M–H]– | 0.40 | 262.60 | 475.1809,193.0512,175.0398,160.0169 | Martynoside | RR |
| 119 | 24.90 | C36H60O11 | 599.1771[M–H]– | 0.10 | 223.97 | 645.1801,551.1576,477.1398,447.1293,281.0661 | Mudanpioside C | PRA |
| 120 | 25.17 | C24H26O9 | 459.1663[M+H]+ | 2.90 | 211.56 | 279.0937,253.0868,163.0391 | Pratensein-7-β-D-glucoside | AR |
| 121\* | 25.56 | C16H12O5 | 285.0748[M+H]+ | –3.30 | 161.68 | 270.0533,253.0488,225.0557,213.0545,197.0603,137.0226 | Calycosin | AR,GRR |
| 122 | 25.80 | C23H28O10 | 463.1609[M–H]– | –0.10 | 216.51 | 509.1661,301.1075,286.0841,271.0608 | Astraisoflavan-7-O-β-D-glucoside | AR |
| 123 | 25.82 | C22H26O8 | 441.1522[M+Na]+ | 0.60 |  | 401.1606,368.1253,247.0972 | Syringaresinol | CR |
| 124 | 25.90 | C21H34O10 | 445.2078[M–H]– | –0.20 | 217.24 | 491.2133,345.1184,179.0546 | Frehmaglutin C | RR |
| 125 | 26.26 | C21H34O10 | 651.2291[M–H]– | –0.40 | 235.81 | 475.1805,193.0512,175.0392,160.0170 | Isomartynoside | RR |
| 126 | 26.53 | C42H66O14 | 795.4566[M+H]+ | 1.30 | 300.05 | 601.4096,503.3363,485.3269,467.3159,439.3580 | Huangqiyenins E | AR |
| 127 | 26.69 | C12H12O2 | 189.0911[M+H]+ | 0.50 |  | 171.0805,161.0965,143.0859,128.0621,115.0546,105.0698 | E-butylidenephthalide | ASR,C |
| 128 | 26.74 | C17H14O6 | 315.0865[M+H]+ | 0.60 | 169.76 | 300.0626,255.0654,243.0657 | Kumatakenin | AR |
| 129 | 27.08 | C20H18O5 | 337.1075[M–H]– | –2.00 | 189.23 | 295.0601,267.0659,171.0061 | Lupiwighteone | GRR |
| 130\* | 28.21 | C12H8O4 | 217.05[M+H]+ | 1.90 | 139.85 | 202.0266,174.0312 | 8-Methoxypsoralen | ASR |
| 131 | 28.28 | C42H64O16 | 825.4240[M+H]+ | –3.20 | 289.42 | 649.3952,455.3508 | Licorice saponin J2 or its isomer | GRR |
| 132 | 28.36 | C21H22O4 | 339.1598[M+H]+ | 2.00 | 184.02 | 297.1121,271.0972,177.0910,145.0647 | Licochalcone A | GRR |
| 133 | 28.38 | C42H64O16 | 823.4124[M–H]– | 0.20 | 290.68 | 653.3371,483.2383,351.0564 | Licorice saponin J2 or its isomer | GRR |
| 134 | 28.47 | C15H12O5 | 273.0761[M+H]+ | 1.10 | 161.86 | 231.0654,153.0184 | Naringenin | GRR |
| 135 | 28.50 | C35H36O15 | 697.2132[M+H]+ | 0.70 | 266.19 | 261.0761,257.0814,233.0647 | Licorice glycoside A | GRR |
| 136 | 28.78 | C16H14O5 | 287.0913[M+H]+ | –0.30 | 161.81 | 269.0808,254.0600,217.0527,135.0435 | Pabulenol | ASR |
| 137 | 29.21 | C48H72O22 | 999.4411[M–H]– | 3.20 |  | 837.3929,485.3256,418.1885,351.0528 | 24-OH Licorice saponin A3 | GRR |
| 138 | 29.28 | C16H14O4 | 271.0962[M+H]+ | –1.00 | 165.87 | 229.0861,177.0541,145.0289,121.0285,107.0496 | Medicarpin | AR |
| 139\* | 29.35 | C30H32O12 | 607.1790[M+H]+ | 0.60 | 236.22 | 585.1996,312.0753,249.0760,151.0755,105.0334 | Benzoyl paeoniflorin | PRA |
| 140 | 29.44 | C17H16O6 | 317.1022[M+H]+ | 0.80 | 169.92 | 339.0853,299.0937 | Homoferreirin | AR |
| 141 | 29.83 | C44H64O19 | 895.3931[M–H]– | –4.20 | 318.73 | 821.3967,629.1887,583.1834,351.0576 | 22-Acetoxyl licorice saponin G2 | GRR |
| 142 | 29.86 | C30H32O12 | 585.1965[M+H]+ | –0.30 | 233.62 | 607.1783,319.1175,301.1064,197.0807,151.0751,105.0332,77.0383 | Benzoyl albiflorin | PRA |
| 143 | 30.00 | C42H62O18 | 855.4009[M+H]+ | 0.00 |  | 877.3828,679.3715,543.1301,503.3378,485.3267,467.3176 | 22 Hydroxy licorice saponin G2 | GRR |
| 144 | 30.17 | C42H66O13 | 779.4576[M+H]+ | –0.10 | 297.25 | 585.418,439.3568 | Licorice saponin C2 | GRR |
| 145 | 30.57 | C44H64O19 | 897.4122[M+H]+ | 0.90 | 319.91 | 703.3680,545.3483,527.3389,509.3269 | Uralsaponin F | GRR |
| 146 | 31.02 | C48H72O21 | 985.4667[M+H]+ | 2.80 | 321.79 | 809.4331,647.3796,615.3896,471.3475,453.3369,435.3255 | Licorice saponin A3 | GRR |
| 147 | 31.08 | C47H78O19 | 947.5215[M+H]+ | 0.50 | 319.88 | 969.5029,437.3412,419.3289 | Astragaloside V | AR |
| 148 | 31.44 | C44H64O19 | 855.4044[M+H]+ | 4.00 |  | 877.3836,503.3378,485.3267,469.3314,376.2285 | Dihydroxy glycyrrhizic acid | GRR |
| 149 | 31.74 | C42H60O17 | 835.3744[M–H]– | 1.60 |  | 857.3856,823.4119,351.0576 | 24-OH Licorice saponin E2 | GRR |
| 150 | 31.87 | C44H64O18 | 881.4187[M+H]+ | 1.20 | 317.94 | 903.3985,705.3853,529.3523,511.3436,460.1876 | 22β-Acetoxy glycyrrhizin | GRR |
| 151 | 32.24 | C42H62O17 | 839.4077[M+H]+ | 2.00 | 297.28 | 663.3747,487.3422,469.3321,451.3209 | Hydroxy glycyrrhizic acid/Macedonoside A/Uralsaponin N/Uralsaponin U | GRR |
| 152 | 32.34 | C36H60O11 | 691.4054[M+Na]+ | 3.70 |  | 633.4012,619.4221,601.4095,473.3619,455.3527,439.3573,437.3412 | Mongholicoside B | AR |
| 153 | 32.38 | C18H20O6 | 333.1332[M+H]+ | 0.00 | 174.53 | 355.1161,184.0998,167.0707,147.0443,137.0598 | Paeonidangenin | PRA |
| 154\* | 32.51 | C15H12O4 | 255.0659[M–H]– | –1.40 | 159.90 | 135.0082,119.0500,91.0182 | Isoliquiritigenin | GRR |
| 155\* | 32.84 | C16H12O4 | 269.0810[M+H]+ | 0.60 | 157.88 | 291.0629,253.0498,237.0550,163.0390 | Formononetin | AR,GRR |
| 156 | 33.11 | C42H58O18 | 851.3708[M+H]+ | 1.40 | 306.06 | 481.2977,463.2873,453.3356 | Uralsaponin D | GRR |
| 157 | 33.40 | C12H14O3 | 205.0869[M–H]– | –0.70 | 164.16 | 189.0552,161.0970,106.0419 | 4-Hydroxy-3-Butylphthalide | ASR,C |
| 158 | 33.42 | C36H60O10 | 675.4087[M+H]+ | 1.20 |  | 487.3433,469.3314,437.3419 | Huangqiyenins B | AR |
| 159 | 33.44 | C47H78O19 | 991.5122[M+HCOO]- | 0.30 | 329.58 | 945.5047,927.4900 | Astragaloside VII | AR |
| 160 | 33.45 | C49H76O19 | 969.5034[M+H]+ | –2.00 | 300.07 | 471.3437,455.3512,437.3411 | Astraisoolesaponins D | AR |
| 161 | 33.55 | C17H16O5 | 301.1064[M+H]+ | –2.20 | 173.68 | 270.0854,191.0707,167.0701,152.0468 | Methylnissolin | AR |
| 162 | 33.81 | C42H60O16 | 819.3804[M–H]– | –0.60 | 286.74 | 351.0567 | Licorice saponin E2 | GRR |
| 163 | 33.86 | C44H66O18 | 883.4346[M+H]+ | 2.70 | 314.15 | 905.4193,645.3629,495.3465,461.1945,451.3233 | 22-Acetoxyl licorice saponin J2 | GRR |
| 164 | 34.10 | C42H62O17 | 839.4080[M+H]+ | 2.50 | 304.44 | 645.3637,487.3426,469.3319,451.3209,439.3216 | Licorice saponin G2 | GRR |
| 165\* | 34.52 | C17H18O5 | 303.1222[M+H]+ | –1.80 | 169.27 | 269.0811,167.0704,152.0649,133.0649,123.0442 | 7,2'-Hydroxy-3',4'-dimethoxyisoflavan | AR |
| 166 | 34.55 | C44H64O17 | 863.4069[M–H]– | –0.10 |  | 351.0541 | 22-Acetoxyl licorice saponin C2 | GRR |
| 167\* | 34.65 | C41H68O14 | 807.4519[M+H]+ | 2.20 | 271.90 | 473.3635,455.3540,437.3411,419.3307 | Astragaloside IV | AR |
| 168 | 34.83 | C42H62O17 | 839.4071[M+H]+ | 1.30 | 305.20 | 645.3633,487.3422,469.3316,451.3205 | Hydroxy glycyrrhizic acid/Macedonoside A/Uralsaponin N/Uralsaponin U | GRR |
| 169\* | 34.91 | C41H68O14 | 807.4503[M+H]+ | 0.30 | 281.57 | 455.3513,437.3413,423.3258,419.3302 | Astragaloside III | AR |
| 170\* | 35.26 | C52H84O21 | 1067.5412[M+Na]+ | 1.40 | 359.80 | 1045.5607,587.3939 | Jujuboside B | JF |
| 171 | 35.52 | C42H62O17 | 839.4079[M+H]+ | 2.30 | 304.23 | 663.3749,645.3644,487.3424,469.3322,451.3211,439.3212 | Hydroxy glycyrrhizic acid/Macedonoside A/Uralsaponin N/Uralsaponin U | GRR |
| 172 | 35.61 | C12H12O3 | 203.0711[M–H]– | –1.20 | 157.99 | 173.0245,160.0167,145.0293,116.9953 | Senkyunolide C | ASR,C |
| 173 | 35.72 | C17H24O2 | 261.1848[M+H]+ | –0.50 | 168.66 | 233.1538,191.1067,177.0912,163.0756,145.0653,137.0599 | Falcarindiol | ASR |
| 174\* | 35.78 | C42H62O16 | 823.4121[M+H]+ | 1.30 | 294.03 | 845.3927,647.3792,471.3473,453.3369,435.3260,407.3308 | Glycyrrhizic acid | GRR |
| 175 | 35.85 | C21H22O6 | 371.1487[M+H]+ | –0.50 | 188.30 | 315.0861,237.1493,201.0468 | Sigmoidin B 3'-methyl ether | GRR |
| 176 | 35.75 | C21H20O6 | 369.1334[M+H]+ | 0.50 | 189.78 | 341.1389,313.0780,285.0759,270.0530,213.0571 | Glycyrrhisoflavanone | GRR |
| 177 | 36.46 | C51H82O21 | 1031.5426[M+H]+ | 0.40 | 318.43 | 647.3790,471.3469,453.3360,451.3221,435.3264,300.2895 | Agroastragalosides Ⅲ | AR |
| 178 | 36.74 | C42H62O17 | 839.4074[M+H]+ | 1.70 | 306.52 | 663.3744,487.3423,469.3318,451.3211,439.3226 | Hydroxy glycyrrhizic acid/Macedonoside A/Uralsaponin N/Uralsaponin U | GRR |
| 179 | 36.92 | C42H64O15 | 809.4311[M+H]+ | 0.80 | 293.06 | 831.4162,633.4016,457.360,439.3583 | Licorice saponin B2 | GRR |
| 180\* | 36.93 | C17H26O4 | 317.1722[M+H]+ | –0.30 | 172.84 | 177.0911,137.0598,122.0365 | 6-Gingerol | ZRR |
| 181 | 37.03 | C48H76O19 | 955.4880[M–H]– | –2.90 | 330.40 | 497.1128 | Yunganoside A1 | GRR |
| 182 | 37.32 | C48H78O18 | 943.5259[M+H]+ | –0.20 | 334.36 | 965.5080,797.4685,617.4074,599.3951,581.3838,441.3728,423.3627,405.3520 | Soyasaponin Ⅰ | AR |
| 183 | 37.37 | C42H62O16 | 823.4118[M+H]+ | 0.90 | 303.65 | 647.3792,453.3362,435.3263,407.3313 | Licorice saponin H2 | GRR |
| 184\* | 37.98 | C12H16O2 | 193.1223[M+H]+ | –0.10 | 163.65 | 215.1042,175.1119,147.1169,119.0856,105.0698,77.0383 | Senkyunolide A | ASR,C |
| 185 | 38.03 | C42H62O16 | 823.4121[M+H]+ | 1.30 | 302.82 | 845.3937,435.3255,407.3312 | Licorice saponin K2 | GRR |
| 186 | 38.38 | C47H76O17 | 913.5173[M+H]+ | 1.90 | 331.61 | 935.4952,599.3946,518.3242,476.2373,423.3643 | Soyasaponin ⅠI | AR |
| 187\* | 38.56 | C43H70O15 | 871.4693[M+HCOO]– | –0.50 | 315.88 | 661.3586,521.3076,492.2725 | Isoastragaloside II | AR |
| 188 | 38.71 | C41H62O14 | 779.4241[M+H]+ | 3.70 | 291.17 | 801.4047,647.3803,471.3476,453.3367 | Araboglycyrrhizin | GRR |
| 189 | 38.74 | C42H64O16 | 825.4281[M+H]+ | 1.70 | 304.23 | 847.4088,631.2834,613.3739,455.3508,437.3417,397.3111 | Uralsaponin C | GRR |
| 190\* | 39.01 | C12H14O2 | 191.1066[M+H]+ | –0.40 | 201.57 | 173.0964,145.1014,117.0699 | 3-Butylphthalide | ASR,C |
| 191 | 39.23 | C42H68O14 | 795.4537[M–H]– | 0.00 | 314.32 | 518.2867 | Astraisoolesaponins A | AR |
| 192 | 39.44 | C20H20O6 | 357.1336[M+H]+ | 1.00 | 183.73 | 301.0714,283.0608,175.0397,147.0446 | Sigmoidin B | GRR |
| 193 | 39.50 | C21H20O6 | 369.133[M+H]+ | –0.70 | 190.22 | 313.0708,285.0764,271.0601,243.0656,191.1070 | Glycycoumarin | GRR |
| 194 | 40.00 | C20H16O6 | 353.1020[M+H]+ | 0.20 | 186.40 | 335.0914,227.0693,153.0185 | Licoisoflavone B its isomer | GRR |
| 195 | 40.21 | C21H22O5 | 355.1538[M+H]+ | –0.60 | 188.31 | 299.0910,165.0553 | Licochalcone D | GRR |
| 196 | 40.63 | C48H76O18 | 941.5127[M+H]+ | 2.40 | 334.18 | 963.4934,597.3785,534.3195,439.3562,421.3448 | Dehydrosoyasaponin I | AR |
| 197 | 40.92 | C17H14O4 | 283.0963[M+H]+ | –0.70 | 164.43 | 267.0657 | 4',7-Dimethoxyisoflavone | AR |
| 198 | 41.65 | C42H62O16 | 823.4111[M+H]+ | 0.10 | 303.06 | 611.3615,453.3359,435.3268,407.3299 | Uralsaponin B/Uralsaponin A | GRR |
| 199 | 41.80 | C43H72O16 | 867.4741[M+H]+ | 3.20 |  | 471.3487,453.3369 | Agroastragaloside Ⅴ | AR |
| 200 | 41.83 | C41H62O14 | 777.4057[M–H]– | –1.30 | 303.03 | 627.3544 | Apioglycyrrhizin | GRR |
| 201 | 42.01 | C20H18O6 | 355.1177[M+H]+ | 0.10 | 184.62 | 337.1076,309.1134,285.0756,269.0451,179.0342 | Isolicoflavonol | GRR |
| 202 | 42.17 | C42H62O16 | 823.4126[M+H]+ | 1.90 | 303.94 | 611.3603,453.3369,435.3261,407.3316 | Uralsaponin B/Uralsaponin A | GRR |
| 203\* | 42.25 | C45H72O16 | 891.4749[M+H]+ | 3.20 | 313.92 | 671.4213,653.4101,549.0821,455.3581,437.3437,419.3318,346.3324,279.0959 | Astragaloside I | AR |
| 204 | 42.29 | C20H18O6 | 353.1027[M–H]– | –1.00 | 189.26 | 284.0325,201.0925 | 5'-(3-Methyl-2-butenyl)-3',4',5,7-tetrahydroxyisoflavone | AR |
| 205 | 42.56 | C12H18O2 | 195.1380[M+H]+ | 0.40 |  | 177.1276,149.1327,121.1007,107.0854 | Neocnidilide | C |
| 206 | 42.76 | C18H18O5 | 315.1227[M+H]+ | 0.20 | 178.64 | 337.1055,167.0706 | P-hydroxyphenethyl ferulate | ASR |
| 207\* | 42.84 | C12H14O2 | 191.1067[M+H]+ | 0.00 | 142.38 | 163.1132,155.0841,145.1009,128.0617,115.0549 | Z-ligustilide | ASR,C |
| 208 | 42.99 | C20H18O6 | 355.1179[M+H]+ | 1.00 | 181.73 | 299.0555,284.0692,271.0606,243.0665 | Licoflavonol | GRR |
| 209 | 43.02 | C26H28O6 | 437.1938[M+H]+ | –2.20 | 204.39 | 419.1857,405.1705,353.1027 | Kanzonol K | GRR |
| 210 | 43.17 | C20H18O5 | 339.1235[M+H]+ | 2.40 | 181.73 | 283.0605,241.0523,149.0606 | Licoflavanone | GRR |
| 211 | 43.28 | C42H66O14 | 793.4373[M–H]– | –0.90 | 317.05 | 613.3756,569.3819,485.3264 | Huangqiyenins E | AR |
| 212 | 43.33 | C20H18O5 | 339.1229[M+H]+ | 0.60 | 187.02 | 283.0600,271.0605,255.0656 | Licoflavone C | GRR |
| 213\* | 43.39 | C45H72O16 | 891.4741[M+H]+ | 3.20 | 226.25 | 671.4179,653.4068,549.0821,437.1952,419.3344,279.0938 | Isoastragaloside I | AR |
| 214 | 43.48 | C21H18O6 | 367.1169[M+H]+ | –1.90 |  | 311.0557,296.0317 | Glycyrol | GRR |
| 215 | 44.41 | C30H46O6 | 501.3222[M–H]– | 0.00 | 226.59 | 457.3331,439.3214 | Glutinosalactone A | RR |
| 216 | 44.62 | C29H44O4 | 455.3162[M–H]– | –1.00 | 220.87 | 441.2997 | 30-Norhederagenin | PRA |
| 217\* | 44.72 | C19H30O4 | 345.2037[M+H]+ | 0.30 | 182.17 | 287.2009,189.0917,177.0913,150.0679,137.0599,122.0365 | 8-Gingerol | ZRR |
| 218 | 44.99 | C12H14O2 | 191.1067[M+H]+ | 0.20 | 201.13 | 173.0964,163.1120,149.0601,145.1014,135.0442,117.0697,105.0699 | E-Ligustilide | ASR,C |
| 219 | 45.22 | C20H16O6 | 353.1020[M+H]+ | 0.00 | 184.00 | 335.0922,299.0552,153.0179 | Licoisoflavone B | GRR |
| 220 | 46.61 | C30H46O5 | 485.3270[M–H]– | –0.40 | 222.79 | 531.3325,467.3156,441.3364,423.3237,405.3161 | Epiceanothic acid | RR |
| 221 | 47.30 | C47H74O17 | 933.4833[M+H]+ | 1.60 | 333.22 | 713.4292,695.4215,437.3412 | Acetylastragaloside Ⅰ | AR |
| 222 | 48.00 | C25H28O6 | 425.1962[M+H]+ | 0.70 | 214.73 | 369.1346,313.0712,301.0729,191.1068,137.0601 | Sigmoidin A | GRR |
| 223 | 48.01 | C25H28O6 | 425.1956[M+H]+ | –0.60 | 208.30 | 369.1334,313.0704,301.0727,179.0342,139.0385 | Gancaonin E | GRR |
| 224 | 48.37 | C30H48O4 | 471.3483[M–H]– | 0.70 | 227.07 | 517.3533,281.2483,239.2026 | 23-Hydroxybetulinic acid | PRA,GRR |
| 225 | 48.46 | C17H24O3 | 299.1621[M+H]+ | 1.10 | 174.41 | 277.1806,221.1178,203.1074,165.0551 | 6-Shogaol | ZRR |
| 226 | 48.76 | C24H28O4 | 381.2063[M+H]+ | 0.70 | 194.99 | 363.1955,335.2001,279.1384,237.0919,191.1067 | Tokinolide B | ASR,C |
| 227 | 49.15 | C24H30O4 | 383.2216[M+H]+ | –0.30 | 190.82 | 405.2034,365.2123,191.1067,135.0441 | Senkyunolide P | ASR,C |
| 228 | 49.28 | C25H26O6 | 423.1800[M+H]+ | –0.60 | 215.34 | 367.1174,311.0551,299.0555 | Sigmoidin F | GRR |
| 229 | 49.41 | C15H22O | 219.1742[M+H]+ | –0.50 | 156.50 | 203.1432,120.0884 | 2-Methyl-6-(4-methylphenyl)-3-heptanone | CR |
| 230\* | 49.58 | C21H34O4 | 373.2348[M+H]+ | –0.30 | 191.28 | 315.2313,277.2162,177.0911,137.0599 | 10-Gingerol | ZRR |
| 231 | 50.49 | C16H22O4 | 301.1409[M+H]+ | –0.40 |  | 279.1594,165.0136,149.0235,135.0439,121.0286 | Dibutyl phthalate | PRA |
| 232\* | 50.64 | C30H46O4 | 471.3477[M+H]+ | 0.80 | 229.59 | 453.3381 | Glycyrrhetinic acid | GRR |
| 233 | 50.92 | C30H46O4 | 469.3325[M–H]– | 0.30 | 221.56 | 515.9632,451.3215,425.3422,407.3319 | Astrantiagenin D | AR |
| 234 | 51.19 | C30H44O4 | 467.3166[M–H]– | –0.10 | 221.80 | 421.3101,337.2115 | Glabrolide | GRR |
| 235 | 51.46 | C24H28O4 | 403.1878[M+Na]+ | –0.50 | 197.99 | 381.2059,363.1954,335.1994,293.1538,191.1067 | Angelicide | ASR,C |
| 236\* | 51.62 | C24H28O4 | 381.2059[M+H]+ | –0.20 | 194.20 | 403.1879,365.2112,213.0889,191.10666,149.0599 | Levistolide A | ASR,C |