**Supplementary data**

# An Integrated Strategy for Global Qualitative and Quantitative Profiling of Traditional Chinese Medicine Formulas: *Baoyuan* Decoction as a Case

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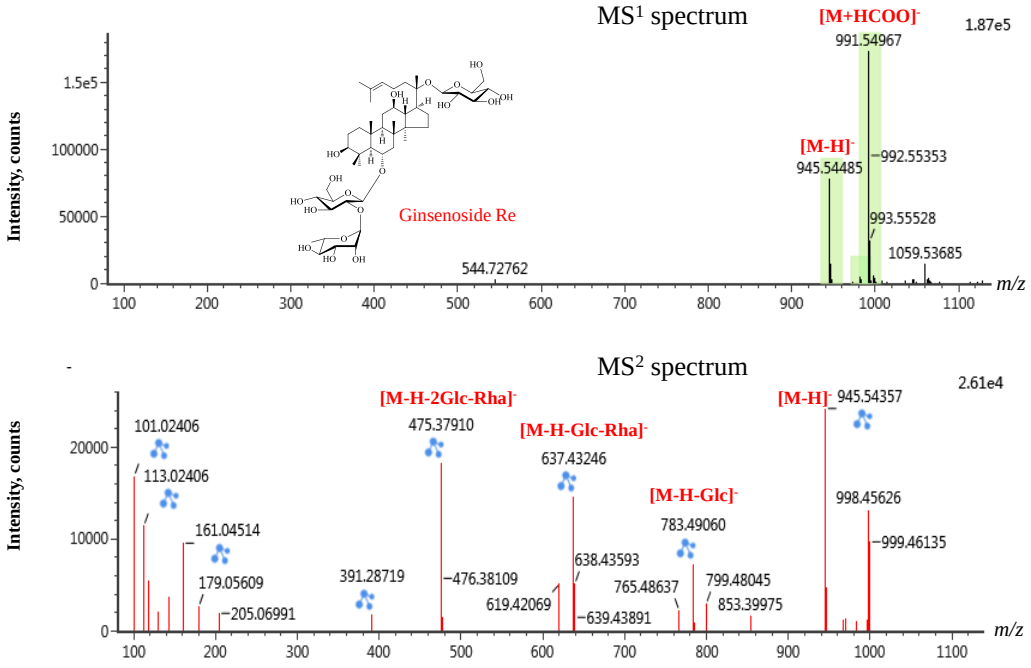



**Figure S1 The accurate MS and MS/MS spectra and the chemical structure of ginsenoside Re.** The signals either highlighted in green or tagged in blue were chosen by UNIFI for rapid structural identification.

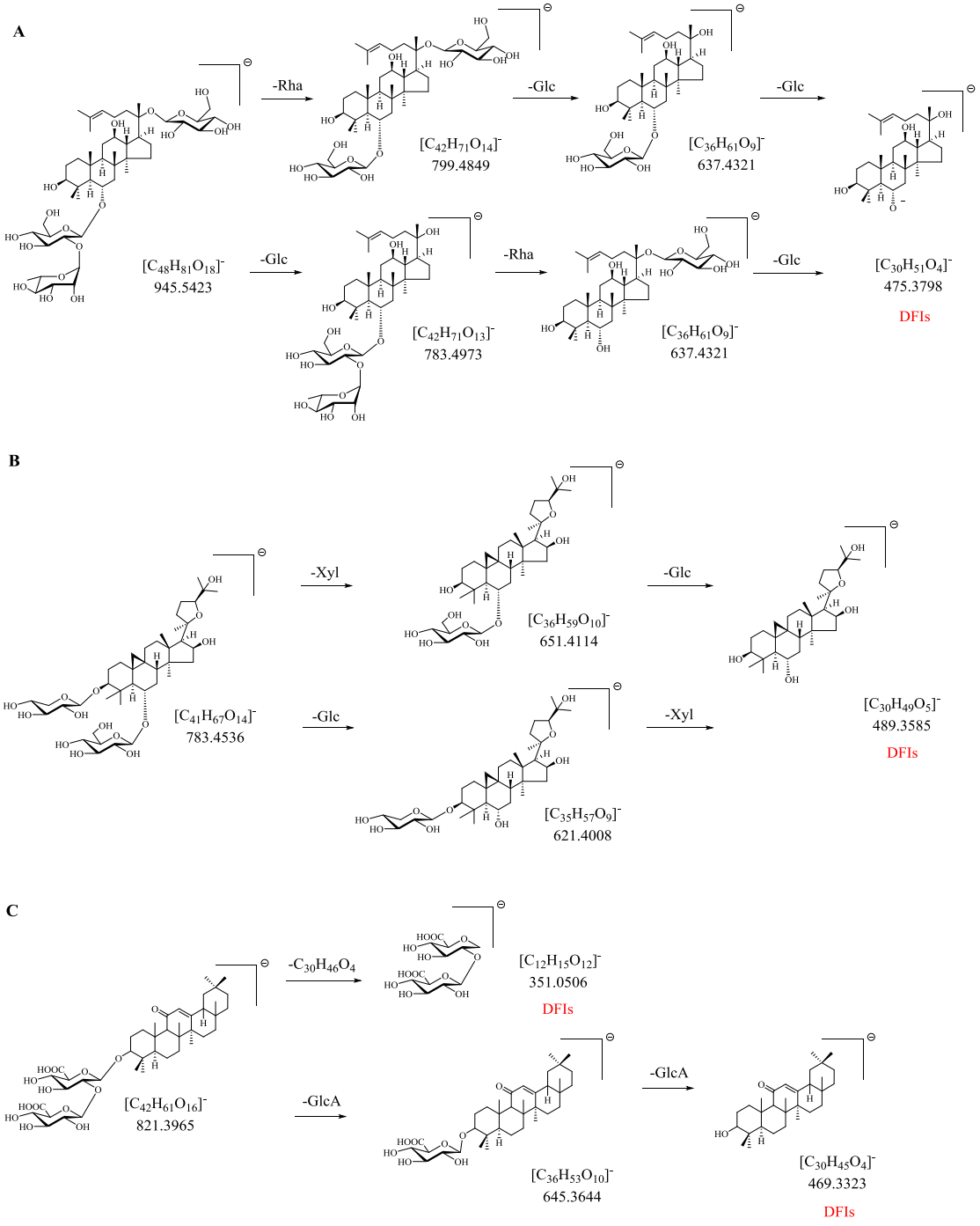



**Figure S2 The proposed fragmentation pathways and main diagnostic fragment ions (DFIs) for ginsenoside Re (A), astragaloside IV (B), and glycyrrhizic acid (C).**

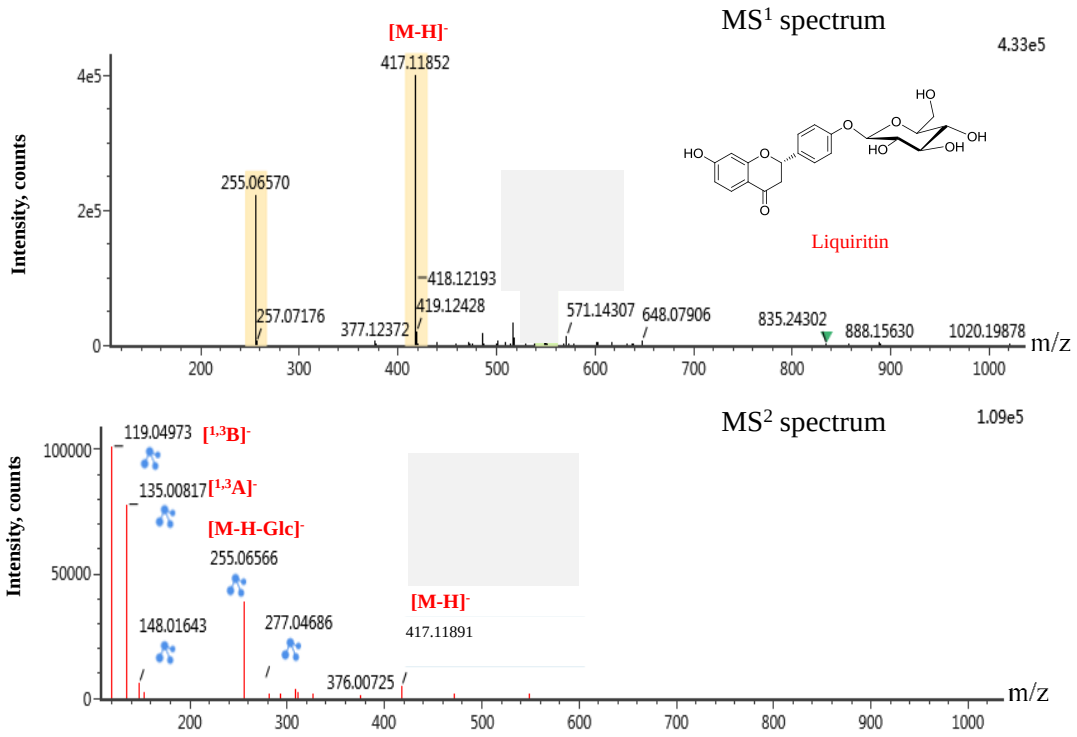



**Figure S3 The accurate MS and MS/MS spectra and the chemical structure of liquiritin**. The signals either highlighted in yellow or tagged in blue were chosen by UNIFI for rapid structural identification.

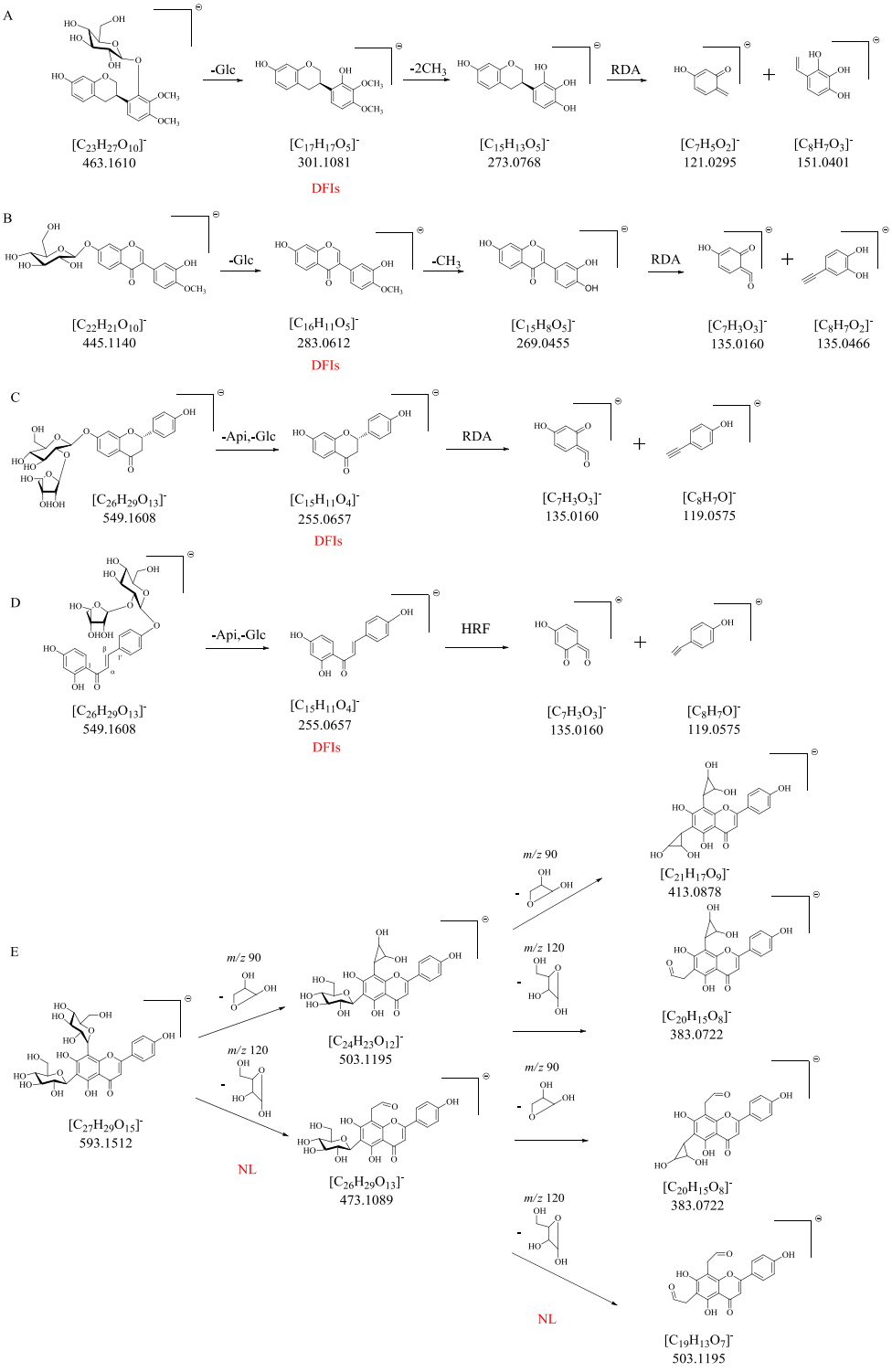
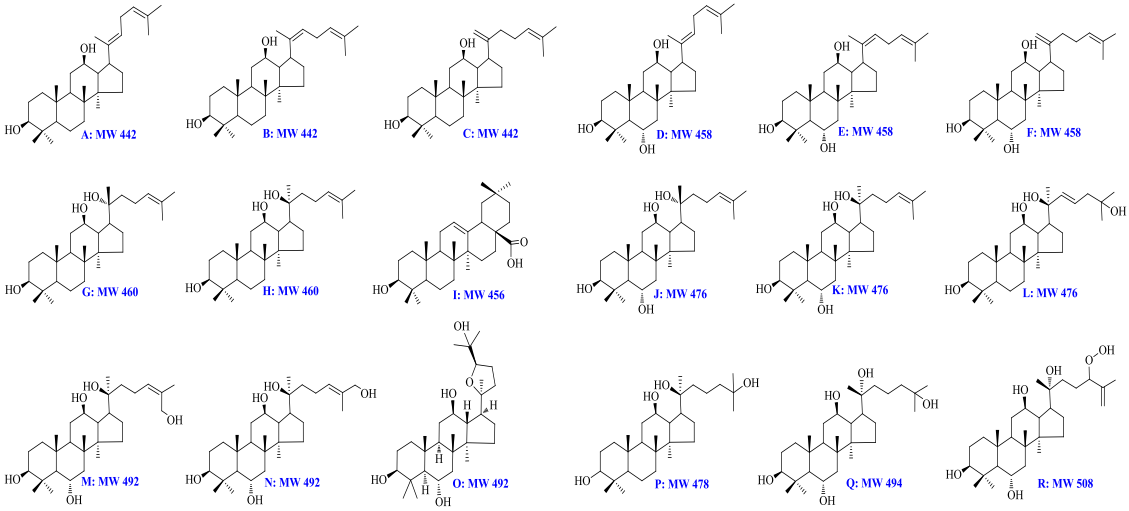
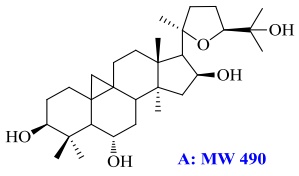



**Figure S4 The proposed fragmentation pathways and primary diagnostic fragment ions (DFIs) for liquiritin apioside (A), isoliquiritin apioside (B), calycosin-7-*O*-*β*-D-glucoside (C), (3*R*)-(+)- isomucronulatol-2′-*O*-*β*-D-glucopyranoside (D), and apigenin-6,8-di-*C*-*β*-D-glucopyranoside (E).**

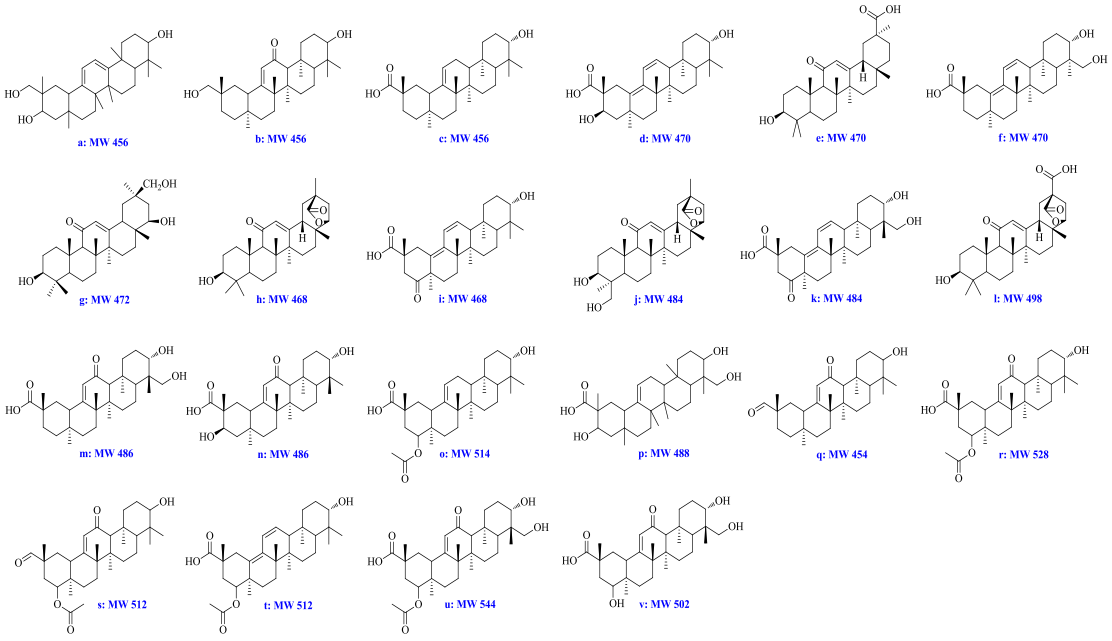
## The aglycones of ginsenosides:




## The aglycone of astragalosides:




## The aglycones of licorice saponins:



**The aglycones of flavonoids:**

| Aglycone | *m/z* | Predictive formula | Characteristic fragments | Group | OH | $OCH_3$ |
|---|---|---|---|---|---|---|
| FA-1 | 255.0663 | $C_{15}H_{11}O_4$ | 135.01,119.05 | I | 2 | 0 |
| FA-2 | 271.0612 | $C_{15}H_{11}O_5$ | 151.00,119.05 | I | 3 | 0 |
| FA-3 | 253.0506 | $C_{15}H_9O_4$ | 135.02,117.04 | II | 2 | 0 |
| FA-4 | 267.0663 | $C_{16}H_{11}O_4$ | 252.04,193.05,135.01 | II | 1 | 1 |
| FA-5 | 269.0455 | $C_{15}H_9O_5$ | 151.00,117.03 | II | 3 | 0 |
| FA-6 | 269.0814 | $C_{16}H_{13}O_4$ | 270.05, 119.05 | I | 2 | 1 |
| FA-7 | 283.0612 | $C_{16}H_{11}O_5$ | 268.03,193.05,135.01 | II | 2 | 1 |
| FA-8 | 285.0612 | $C_{16}H_{11}O_5$ | 270.05,119.05 | I | 2 | 1 |
| FA-9 | 289.0712 | $C_{15}H_{13}O_6$ | 137.0238,109.0196 | III | 5 | 0 |
| FA-10 | 299.0561 | $C_{16}H_{11}O_6$ | 284.03,135.02 | II | 3 | 1 |
| FA-11 | 299.0925 | $C_{17}H_{15}O_5$ | 284.07,269.04 | IV | 1 | 2 |
| FA-12 | 301.1099 | $C_{17}H_{17}O_5$ | 271.06,193.05,135.05 | III | 3 | 2 |

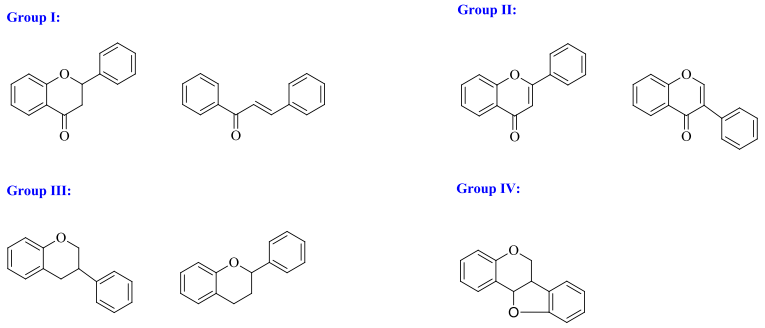



**Figure S5 The common aglycones of ginsenosides, astragalosides, licorice saponins, and flavonoids in BYD.**

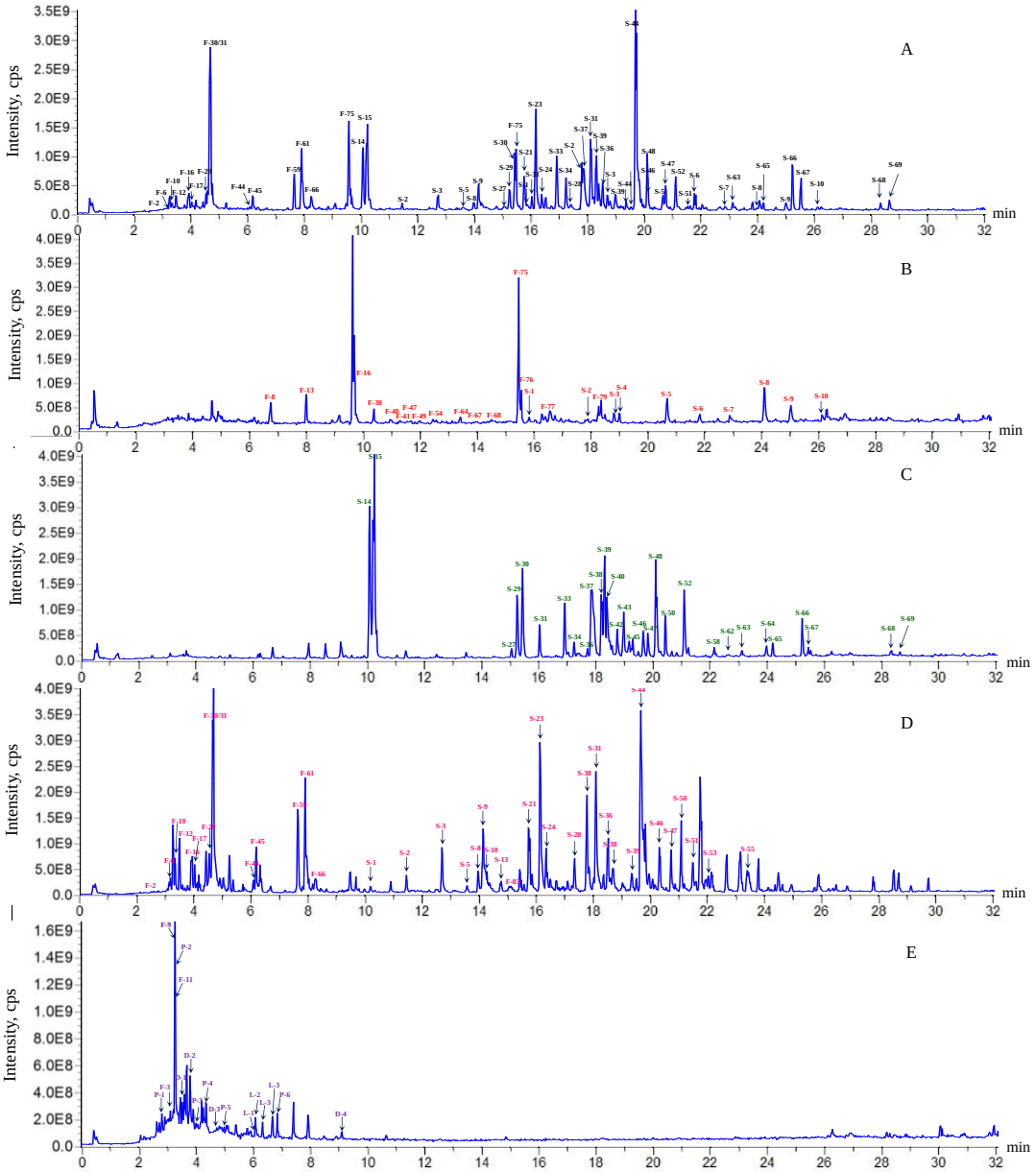



**Figure S6 The base peak chromatograms (BPCs) of *Baoyuan* decoction extract (A), Astragali Radix extract (B), Ginseng Radix extract (C), Glycyrrhiza Radix et Rhizoma Praeparata Cum Melle extract (D), and Cinnamomi Cortex extract (E) by UPLC/Qtrap-MS in negative mode.**

**Table S1 The MS/MS spectral data of chemical constituents of *Baoyuan* decoction by UPLC/Q-TOF-MS.**

| No. | $t_R$ (min) | [Aglycone-H]$^-$ | Fragment ions |
|---|---|---|---|
| $S_{GU}$-1$^m$ | 9.5 | p [M-H-2GlcA]$^-$ | 663.3879 [M-H-GlcA]$^-$, 351.0556 [2GlcA-H]$^-$ |
| $S_{GU}$-2$^m$ | 10.94 | g [M-H-2GlcA-Rha]$^-$ | 793.4360 [M-H-GlcA]$^-$, 617.3657 [M-H-2GlcA]$^-$, 471.3477 [M-H-2GlcA-Rha]$^-$, 351.0558 [2GlcA-H]$^-$ |
| $S_{GU}$-3*$^C$ | 12.2 | g [M-H-2GlcA]$^-$ | 647.3791 [M-H-GlcA]$^-$, 471.3448 [M-H-2GlcA]$^-$, 351.0563 [2GlcA-H]$^-$ |
| $S_{GU}$-4$^m$ | 12.33 | g [M-H-2GlcA-Rha]$^-$ | 823.4045 [M-H-Rha]$^-$, 471.3477 [M-H-2GlcA-Rha]$^-$, 351.0558 [2GlcA-H]$^-$ |
| $S_{GU}$-5$^m$ | 12.82 | g [M-H-2GlcA-Glc- $C_2H_2O$]$^-$ | 985.4524 [M-H-$C_2H_2O$]$^-$, 823.3965 [M-H-$C_2H_2O$-Glc]$^-$, 471.3505 [M-H-2GlcA-Glc-$C_2H_2O$]$^-$, 351.0581 [2GlcA-H]$^-$ |
| $S_{GU}$-6$^C$ | 12.97 | j/k [M-H-2GlcA]$^-$ | 659.3494 [M-H-GlcA]$^-$, 483.3309 [M-H-2GlcA]$^-$, 351.0563 [2GlcA-H]$^-$ |
| $S_{GU}$-7$^m$ | 13.06 | g [M-H-2GlcA]$^-$ | 647.3791 [M-H-GlcA]$^-$, 471.3448 [M-H-2GlcA]$^-$, 351.0563 [2GlcA-H]$^-$ |
| $S_{GU}$-8$^m$ | 13.4 | m/n [M-H-2GlcA-Gic]$^-$ | 837.3893 [M-H-Glc]$^-$, 661.3572 [M-H-GlcA-Glc]$^-$, 485.3264 [M-H-2GlcA-Glc]$^-$, 351.0562 [2GlcA-H]$^-$ |
| $S_{GU}$-9* | 13.5 | u [M-H-2GlcA]$^-$ | 719.3635 [M-H-GlcA]$^-$, 351.0554 [2GlcA-H]$^-$ |
| $S_{GU}$-10$^C$ | 13.6 | d/e/f [M-H-2GlcA]$^-$ | 645.3670 [M-H-GlcA]$^-$, 469.3323 [M-H-2GlcA]$^-$, 425.3443 [M-H-2GlcA-$CO_2$]$^-$, 351.0577 [2GlcA-H]$^-$ |
| $S_{GU}$-11$^C$ | 13.68 | v [M-H-2GlcA]$^-$ | 501.3202 [M-H-2GlcA]$^-$ |
| $S_{GU}$-12$^m$ | 14.07 | 499.3 [M-H-2GlcA]$^-$ | 851.4082 [M-H-GlcA]$^-$, 499.3202 [M-H-2GlcA]$^-$, 351.0552 [2GlcA-H]$^-$ |
| $S_{GU}$-13$^m$ | 14.13 | u [M-H-2GlcA]$^-$ | 719.3635 [M-H-GlcA]$^-$, 351.0554 [2GlcA-H]$^-$ |
| $S_{GU}$-14$^m$ | 14.17 | d/e/f [M-H-2GlcA-Ara/Xyl]$^-$ | 777.4429 [M-H-GlcA]$^-$, 469.3299 [M-H-2GlcA-Ara/Xyl]$^-$ |
| $S_{GU}$-15$^C$ | 14.38 | g [M-H-2GlcA]$^-$ | 647.3791 [M-H-GlcA]$^-$, 471.3448 [M-H-2GlcA]$^-$, 351.0563 [2GlcA-H]$^-$ |
| $S_{GU}$-16$^m$ | 14.6 | o [M-H-2GlcA-Rha]$^-$ | 951.4619 [M-H-$C_2H_4O_2$]$^-$, 599.3514 [M-H-$C_2H_4O_2$-2GlcA]$^-$,497.1150 [2GlcA·Rha-H]$^-$,467.3169 [M-H-$C_2H_4O$-2GlcA-Rha]$^-$ |

| | | | |
|---|---|---|---|
| $S_{GU}$-17[C] | 15 | j/k [M-H-2GlcA]$^-$ | 659.3494 [M-H-GlcA]$^-$, 483.3130 [M-H-2GlcA]$^-$ |
| $S_{GU}$-18[C] | 15.01 | l [M-H-2GlcA]$^-$ | 497.2903 [M-H-2GlcA]$^-$ |
| $S_{GU}$-19[m] | 15.16 | j/k [M-H-2GlcA]$^-$ | 659.3494 [M-H-GlcA]$^-$, 483.3130 [M-H-2GlcA]$^-$, 351.0554 [2GlcA-H]$^-$ |
| $S_{GU}$-20[C] | 15.22 | r [M-H-3GlcA]$^-$ | 849.3576 [M-H-GlcA]$^-$, 497.1150 [2GlcA·Rha-H]$^-$, 351.0554 [2GlcA-H]$^-$ |
| $S_{GU}$-21*[C] | 15.31 | e [M-H-2GlcA-Glc]$^-$ | 821.3964 [M-H-Glc]$^-$, 645.3637 [M-H-GlcA-Glc]$^-$, 469.3326 [M-H-2GlcA-Glc]$^-$, 351.0565 [2GlcA-H]$^-$ |
| $S_{GU}$-22[m] | 15.75 | r [M-H-GlcA-Glc-$C_2H_2O$]$^-$ | 703.3715 [M-H-Glc]$^-$, 527.3386 [M-H-GlcA-Glc]$^-$, 485.3268 [M-H-GlcA-Glc-$C_2H_2O$]$^-$ |
| $S_{GU}$-23*[C] | 15.87 | r [M-H-2GlcA]$^-$ | 703.3703 [M-H-GlcA]$^-$, 527.3374 [M-H-2GlcA]$^-$, 351.0554 [2GlcA-H]$^-$ |
| $S_{GU}$-24[m] | 16.03 | m/n [M-H-2GlcA]$^-$ | 661.3601 [M-H-GlcA]$^-$, 485.3268 [M-H-2GlcA]$^-$, 351.0559 [2GlcA-H]$^-$ |
| $S_{GU}$-25[m] | 16.26 | m/n [M-H-2Glc-Xyl]$^-$ | 617.3721 [M-H-2GlcA]$^-$, 485.3271[M-H-2Glc-Xyl]$^-$, 351.0558 [2GlcA-H]$^-$ |
| $S_{GU}$-26[m] | 16.3 | r [M-H-GlcA-Glc]$^-$ | 703.3715 [M-H-Glc]$^-$, 527.3386 [M-H-GlcA-Glc]$^-$ |
| $S_{GU}$-27[m] | 16.37 | m/n [M-H-2GlcA-Ara/Xyl]$^-$ | 617.3721 [M-H-2GlcA]$^-$, 485.3271 [M-H-2GlcA-Ara/Xyl]$^-$, 351.0558 [2GlcA-H]$^-$ |
| $S_{GU}$-28[C] | 16.53 | m/n [M-H-GlcA-Glc]$^-$ | 661.3524 [M-H-Glc]$^-$, 485.3271 [M-H-GlcA-Glc]$^-$ |
| $S_{GU}$-29[m] | 16.83 | a/b/c [M-H-2GlcA-Rha]$^-$ | 497.1002 [2GlcA·Rha-H]$^-$ |
| $S_{GU}$-30*[C] | 17.2 | h [M-H-2GlcA]$^-$ | 643.3481 [M-H-GlcA]$^-$, 467.3163 [M-H-2GlcA]$^-$ |
| $S_{GU}$-31*[C] | 17.41 | m [M-H-2GlcA]$^-$ | 661.3601 [M-H-GlcA]$^-$, 485.3268 [M-H-2GlcA]$^-$, 351.0559 [2GlcA-H]$^-$ |
| $S_{GU}$-32[m] | 17.51 | a/b/c [M-H-2GlcA]$^-$ | 631.3805 [M-H-GlcA]$^-$, 455.3443 [M-H-2GlcA]$^-$ |
| $S_{GU}$-33[C] | 17.53 | m/n [M-H-GlcA-Glc]$^-$ | 661.3524 [M-H-Glc]$^-$, 485.3271 [M-H-GlcA-Glc]$^-$ |
| $S_{GU}$-34[m] | 17.75 | m/n [M-H-2GlcA]$^-$ | 661.3524 [M-H-Glc]$^-$, 485.3271 [M-H-GlcA-Glc]$^-$, 351.0559 [2GlcA-H]$^-$ |
| $S_{GU}$-35[C] | 17.78 | h/i [M-H-2GlcA]$^-$ | 643.3510 [M-H-GlcA]$^-$, 467.467.3163 [M-H-2GlcA]$^-$, 351.0559 [2GlcA-H]$^-$ |
| $S_{GU}$-36[m] | 18 | s/t [M-H-2GlcA]$^-$ | 687.3720 [M-H-GlcA]$^-$, 511.3531 [M-H-2GlcA]$^-$, 469.3323 [M-H-2GlcA-$C_2H_2O$]$^-$, 351.0559 [2GlcA-H]$^-$ |

| | | | |
|---|---|---|---|
| $S_{GU}$-37 [m] | 18.12 | d/e/f [M-H-2GlcA-Xyl]$^-$ | 777.4111 [M-H-GlcA]$^-$, 469.3299 [M-H-2GlcA-Xyl]$^-$, 351.0542 [2GlcA-H]$^-$ |
| $S_{GU}$-38 [m] | 18.3 | r [M-H-2GlcA]$^-$ | 703.3664 [M-H-GlcA]$^-$, 527.3397 [M-H-2GlcA]$^-$, 485.3320 [M-H-2GlcA-$C_2H_2O$]$^-$, 351.0565 [2GlcA-H]$^-$ |
| $S_{GU}$-39 [m] | 18.39 | r [M-H-GlcA-Glc]$^-$ | 703.3715 [M-H-Glc]$^-$, 527.3386 [M-H-GlcA-Glc]$^-$, 485.3268 [M-H-2GlcA-$C_2H_2O$]$^-$ |
| $S_{GU}$-40 [m] | 18.48 | 441.3 [M-H-2GlcA]$^-$ | 617.3752 [M-H-GlcA]$^-$, 441.3302 [M-H-2GlcA]$^-$, 351.0577 [2GlcA-H]$^-$ |
| $S_{GU}$-41 [m] | 18.5 | d/e/f [M-H-2GlcA-Rha]$^-$ | 821.3983 [M-H-Rha]$^-$, 645.3670 [M-H-Rha-GlcA]$^-$, 497.1002 [2GlcA-Rha-H]$^-$, 469.3323 [M-H-Rha-2GlcA]$^-$ |
| $S_{GU}$-42[C] | 18.66 | m/n [M-H-2GlcA]$^-$ | 661.3601 [M-H-GlcA]$^-$, 485.3268 [M-H-2GlcA]$^-$, 351.0559 [2GlcA-H]$^-$ |
| $S_{GU}$-43 [m] | 18.75 | o [M-H-2GlcA]$^-$ | 689.3898 [M-H-GlcA]$^-$, 513.3629 [M-H-2GlcA]$^-$ |
| $S_{GU}$-44*[C] | 19.01 | e [M-H-2GlcA]$^-$ | 645.3670 [M-H-GlcA]$^-$, 469.3323 [M-H-2GlcA]$^-$, 351.0577 [2GlcA-H]$^-$ |
| $S_{GU}$-45*[C] | 19.11 | e [M-H-2GlcA]$^-$ | 645.3670 [M-H-GlcA]$^-$, 469.3323 [M-H-2GlcA]$^-$, 351.0577 [2GlcA-H]$^-$ |
| $S_{GU}$-46 [m] | 19.23 | d/e/f [M-H-GlcA-Glc]$^-$ | 631.3822 [M-H-GlcA]$^-$, 469.3297 [M-H-GlcA-Glc]$^-$ |
| $S_{GU}$-47[C] | 19.7 | d/e/f [M-H-GlcA-Glc]$^-$ | 631.3822 [M-H-GlcA]$^-$, 469.3297 [M-H-GlcA-Glc]$^-$ |
| $S_{GU}$-48[C] | 20.01 | a/b/c [M-H-2GlcA]$^-$ | 631.3822 [M-H-GlcA]$^-$, 469.3323 [M-H-2GlcA]$^-$, 351.0577 [2GlcA-H]$^-$ |
| $S_{GU}$-49 [m] | 20.14 | a/b/c [M-H-2GlcA]$^-$ | 631.3822 [M-H-GlcA]$^-$, 469.3323 [M-H-2GlcA]$^-$, 351.0577 [2GlcA-H]$^-$ |
| $S_{GU}$-50 [m] | 20.39 | d/e/f [M-H-2GlcA]- | 645.3670 [M-H-GlcA]$^-$, 469.3323 [M-H-2GlcA]$^-$, 351.0577 [2GlcA-H]$^-$ |
| $S_{GU}$-51[C] | 20.79 | d/e/f [M-H-2GlcA]$^-$ | 645.3670 [M-H-GlcA]$^-$, 469.3323 [M-H-2GlcA]$^-$, 351.0577 [2GlcA-H]$^-$ |
| $S_{GU}$-52 [m] | 21.1 | d/e/f [M-H-GlcA-Glc]$^-$ | 601.3758 [M-H-GlcA]$^-$, 469.3323 [M-H-GlcA-Glc]$^-$ |
| $S_{GU}$-53*[C] | 21.49 | g [M-H-2GlcA]$^-$ | 647.3791 [M-H-GlcA]$^-$, 471.3448 [M-H-2GlcA]$^-$, 351.0563 [2GlcA-H]$^-$ |
| $S_{GU}$-54[C] | 22.5 | q [M-H-2GlcA]$^-$ | 629.3651 [M-H-GlcA]$^-$, 453.3201 [M-H-2GlcA]$^-$, 351.0561 [2GlcA-H]$^-$ |
| $S_{GU}$-55*[C] | 22.98 | c [M-H-2GlcA]$^-$ | 631.3822 [M-H-GlcA]$^-$, 455.3515 [M-H-2GlcA]$^-$, 351.0562 [2GlcA-H]$^-$ |
| $S_{GU}$-56 [m] | 29.59 | e [M-H]$^-$ | 425.3417 [M-H-$CO_2$]$^-$ |

| | | | |
|---|---|---|---|
| $S_{AM}$-1[C] | 15.02 | 489.4 [M-H-2Glc-Xyl]$^-$ | 783.4547 [M-H-Glc]$^-$, 621.4390 [M-H-2Glc]$^-$, 489.3642 [M-H-2Glc-Xyl]$^-$ |
| $S_{AM}$-2[C] | 16.8 | 489.4 [M-H-2Glc-Xyl]$^-$ | 783.4547 [M-H-Glc]$^-$, 621.4390 [M-H-2Glc]$^-$, 489.3642 [M-H-2Glc-Xyl]$^-$ |
| $S_{AM}$-3*[C] | 17.9 | 489.4 [M-H-Glc-Xyl]$^-$ | 489.3587 [M-H-Glc-Xyl]$^-$ |
| $S_{AM}$-4*[C] | 18.1 | 489.4 [M-H-Glc-Xyl]$^-$ | 621.4390 [M-H-Glc]$^-$, 489.3642 [M-H-Glc-Xyl]$^-$ |
| $S_{AM}$-5*[C] | 19.77 | 489.4 [M-H-Ac-Glc-Xyl]$^-$ | 783.4547 [M-H-Ac]$^-$, 621.4390 [M-H-Ac-Glc]$^-$, 489.3642 [M-H-Ac-Glc-Xyl]$^-$ |
| $S_{AM}$-6[C] | 20.89 | 489.4 [M-H-Ac-Xyl-Glc]$^-$ | 783.4547 [M-H-Ac]$^-$, 621.4390 [M-H-Ac-Glc]$^-$, 489.3642 [M-H-Ac-Glc-Xyl]$^-$ |
| $S_{AM}$-7*[C] | 21.92 | 489.4 [M-H-Ac-Glc-Xyl]$^-$ | 783.4547 [M-H-Ac]$^-$, 621.4390 [M-H-Ac-Glc]$^-$, 489.3642 [M-H-Ac-Glc-Xyl]$^-$ |
| $S_{AM}$-8[C] | 23.32 | 489.4 [M-H-2Ac-Glc-Xyl]$^-$ | 871.4691 [M+HCOO-Ac]$^-$, 783.4547 [M-H-2Ac]$^-$, 621.4390 [M-H-2Ac-Glc]$^-$, 489.3642 [M-H-2Ac-Glc-Xyl]$^-$ |
| $S_{AM}$-9*[C] | 24.16 | 489.4 [M-H-2Ac-Glc-Xyl]$^-$ | 871.4691 [M+HCOO-Ac]$^-$, 783.4547 [M-H-2Ac]$^-$, 621.4390 [M-H-2Ac-Glc]$^-$, 489.3642 [M-H-2Ac-Glc-Xyl]$^-$ |
| $S_{AM}$-10[C] | 25.29 | 489.4 [M-H-2Ac-Glc-Xyl]$^-$ | 871.4691 [M+HCOO-Ac]$^-$, 783.4547 [M-H-2Ac]$^-$, 621.4390 [M-H-2Ac-Glc]$^-$, 489.3642 [M-H-2Ac-Glc-Xyl]$^-$ |
| $S_{PG}$-1[m] | 2.79 | Q [M-H-3Glc]$^-$ | 817.5058 [M-H-Glc]$^-$, 799.4803 [M-H-Glc-$H_2O$]$^-$, 655.4559 [M-H-2Glc]$^-$, 637.4381 [M-H-2Glc-$H_2O$]$^-$, 493.3892 [M-H-3Glc]$^-$ |
| $S_{PG}$-2[m] | 3.61 | J/K/L [M-H-3Glc]$^-$ | 799.4847 [M-H-Glc]$^-$, 637.4314 [M-H-2Glc]$^-$, 475.3783 [M-H-3Glc]$^-$, 391.2837 [M-H-3Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-3[m] | 3.65 | J/K/L [M-H-4Glc]- | 799.4847 [M-H-Glc]$^-$, 637.4314 [M-H-2Glc]$^-$, 475.3783 [M-H-3Glc]$^-$, 391.2837 [M-H-3Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-4[m] | 3.86 | Q [M-H-2Glc-Rha]$^-$ | 801.5052 [M-H-Glc]$^-$, 493.3945 [M-H-2Glc-Rha]$^-$ |
| $S_{PG}$-5[m] | 5.22 | M/N/O [M-H-2Glc-Rha]$^-$ | 815.4845 [M-H-Rha]$^-$, 653.4266 [M-H-Glc-Rha]$^-$, 491.3752 [M-H-2Glc-Rha]$^-$ |
| $S_{PG}$-6[m] | 7.02 | J/K/L [M-H-3Glc]$^-$ | 799.4847 [M-H-Glc]$^-$, 637.4314 [M-H-2Glc]$^-$, 475.3783 [M-H-3Glc]$^-$ |
| $S_{PG}$-7[m] | 7.27 | Q [M-H-Glc-Rha]$^-$ | 493.3892 [M-H-3Glc]$^-$ |

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| $S_{PG}$-8[C] | 7.71 | J/K/L [M-H-2Glc-Xyl]$^-$ | 799.4836 [M-H-Xyl]$^-$, 637.4317 [M-H-Glc-Xyl]$^-$, 475.3784 [M-H-2Glc-Xyl]$^-$, 391.2831 [M-H-2Glc-Xyl-$C_6H_{12}$]$^-$ |
| $S_{PG}$-9[C] | 7.74 | J/K/L [M-H-3Glc]$^-$ | 799.4817 [M-H-Glc]$^-$, 637.4340 [M-H-2Glc]$^-$, 475.3737 [M-H-3Glc]$^-$ |
| $S_{PG}$-10[C] | 8.39 | J/K/L [M-H-2Glc-Xyl]$^-$ | 799.4836 [M-H-Xyl]$^-$, 637.4317[M-H-Glc-Xyl]$^-$, 475.3784 [M-H-2Glc-Xyl]$^-$, 391.2831 [M-H-2Glc-Xyl-$C_6H_{12}$]$^-$ |
| $S_{PG}$-11[m] | 8.56 | R [M-H-Glc-Xyl]$^-$ | 639.4144 [M-H-Glc]$^-$, 507.2037 [M-H-Glc-Xyl]$^-$ |
| $S_{PG}$-12[m] | 8.9 | J/K/L [M-H-3Glc]$^-$ | 799.4817 [M-H-Glc]$^-$, 637.4340 [M-H-2Glc]$^-$, 475.3737 [M-H-3Glc]$^-$ |
| $S_{PG}$-13[m] | 9.01 | J/K/L [M-H-3Glc]$^-$ | 799.4817 [M-H-Glc]$^-$, 637.4340 [M-H-2Glc]$^-$, 475.3737 [M-H-3Glc]$^-$ |
| $S_{PG}$-14*[C] | 9.2 | L [M-H-2Glc]$^-$ | 637.4314 [M-H-Glc]$^-$, 475.3783 [M-H-2Glc]$^-$, 391.2837 [M-H-2Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-15*[C] | 9.37 | L [M-H-2Glc-Rha]$^-$ | 783.4855 [M-H-Glc]$^-$, 637.4304 [M-H-Glc-Rha]$^-$, 475.3775 [M-H-2Glc-Rha]$^-$ |
| $S_{PG}$-16[C] | 9.4 | J/K/L [M-H-2Glc]$^-$ | 637.4314 [M-H-Glc]$^-$, 475.3783 [M-H-2Glc]$^-$, 391.2837 [M-H-2Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-17[m] | 9.8 | J/K/L [M-H-2Glc]$^-$ | 637.4314 [M-H-Glc]$^-$, 475.3783 [M-H-2Glc]$^-$, 391.2837 [M-H-2Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-18[m] | 10.12 | J/K/L [M-H-2Glc]$^-$ | 637.4314 [M-H-Glc]$^-$, 475.3783 [M-H-2Glc]$^-$, 391.2837 [M-H-2Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-19[m] | 10.86 | Q [M-H-2Glc-Rha]$^-$ | 817.5058 [M-H-Glc]$^-$, 799.4803 [M-H-Glc-$H_2O$]$^-$, 655.4559 [M-H-2Glc]$^-$, 637.4381 [M-H-2Glc-$H_2O$]$^-$, 493.3875 [M-H-2Glc-Rha]$^-$, 475.3732 [M-H-2Glc-Rha-$H_2O$]$^-$, 375.7589 [M-H-2Glc-Rha-$H_2O$-$C_6H_{12}$]$^-$ |
| $S_{PG}$-20[m] | 10.9 | J/K/L [M-H-Ac-2Glc-Rha]$^-$ | 945.5423 [M-H-Ac]$^-$, 799.4847 [M-H-Ac-Rha]$^-$, 637.4314 [M-H-Ac-Glc-Rha]$^-$, 475.3783 [M-H-Ac-2Glc-Rha]$^-$, 391.2837 [M-H-Ac-2Glc-Rha-$C_6H_{12}$]$^-$ |
| $S_{PG}$-21[m] | 11.5 | J/K/L [M-H-Glc-Rha-Xyl/Ara]$^-$ | 753.4858 [M-H-Glc]$^-$, 607.4185 [M-H-Glc-Rha]$^-$, 475.3782 |

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| | | | [M-H-Glc-Rha-Xyl/Ara]$^-$ |
| $S_{PG}$-22 [m] | 11.63 | J/K/L [M-H-Ac-2Glc-Rha]$^-$ | 945.5423 [M-H-Ac]$^-$, 799.4847 [M-H-Ac-Rha]$^-$, 637.4314 [M-H-Ac-Glc-Rha]$^-$, 475.3783 [M-H-Ac-2Glc-Rha]$^-$ |
| $S_{PG}$-23 [m] | 12.56 | J/K/L [M-H-Glc-Rha-Xyl/Ara]$^-$ | 783.4884 [M-H-Xyl/Ara]$^-$, 637.4296 [M-H-Rha-Xyl/Ara]$^-$, 475.3782 [M-H-Glc-Rha-Xyl/Ara]$^-$ |
| $S_{PG}$-24 [m] | 12.72 | P [M-H-4Glc]$^-$ | 963.5451 [M-H-4Glc]$^-$, 801.4897 [M-H-2Glc]$^-$, 639.4481 [M-H-3Glc]$^-$, 477.4033 [M-H-4Glc]$^-$ |
| $S_{PG}$-25 [m] | 13.09 | J/K/L [M-H-Ac-2Glc-Rha]$^-$ | 945.5423 [M-H-Ac]$^-$, 783.4827 [M-H-Ac-Glc]$^-$, 637.4314 [M-H-Ac-Glc-Rha]$^-$, 475.3783 [M-H-Ac-2Glc-Rha]$^-$, 391.2837 [M-H-Ac-2Glc-Rha-$C_6H_{12}$]$^-$ |
| $S_{PG}$-26 [m] | 13.56 | J/K/L [M-H-3Glc]$^-$ | 799.4817 [M-H-Glc]$^-$, 637.4340 [M-H-2Glc]$^-$, 475.3737 [M-H-3Glc]$^-$ |
| $S_{PG}$-27[C] | 14 | M/N/O [M-H-Glc-Xyl]$^-$ | 653.4175 [M-H-Xyl]$^-$, 491.3735 [M-H-Glc-Xyl]$^-$ |
| $S_{PG}$-28 [m] | 14.24 | Q [M-H-2Glc-Rha]$^-$ | 801.5052 [M-H-Glc]$^-$, 493.3945 [M-H-2Glc-Rha]$^-$ |
| $S_{PG}$-29*[C] | 14.46 | L [M-H-2Glc]$^-$ | 637.4314 [M-H-Glc]$^-$, 475.3783 [M-H-2Glc]$^-$, 391.2837 [M-H-2Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-30*[C] | 14.57 | O [M-H-Rha-Glc]$^-$ | 653.4260 [M-H-Rha]$^-$, 491.3739 [M-H-Rha-Glc]$^-$ |
| $S_{PG}$-31[C] | 15.24 | J/K/L [M-H-Xyl-Glc]$^-$ | 637.4302 [M-H-Xyl]$^-$, 475.3772 [M-H-Xyl-Glc]$^-$, 391.2845 [M-H-Xyl-Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-32[C] | 15.99 | J/K/L [M-H-Glc]$^-$ | 475.3784 [M-H-Glc]$^-$, 391.2850 [M-H-Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-33*[C] | 16.08 | L [M-H-Rha-Glc]$^-$ | 637.4318 [M-H-Rha]$^-$, 475.3784 [M-H-Rha-Glc]$^-$, 391.2850 [M-H-Rha-Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-34[C] | 16.38 | J/K/L [M-H-Rha-Glc]$^-$ | 637.4318 [M-H-Rha]$^-$, 475.3784 [M-H-Rha-Glc]$^-$, 391.2850 [M-H-Rha-Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-35[C] | 16.5 | J/K/L [M-H-Glc]$^-$ | 475.3784 [M-H-Glc]$^-$, 391.2850 [M-H-Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-36 [m] | 16.77 | G/H [M-H-2Xyl-3Glc]$^-$ | 1077.5848 [M-H-Xyl]$^-$,945.5418 [M-H-2Xyl]$^-$, 783.4890 [M-H-2Xyl-Glc]$^-$, 621.4382 [M-H-2Xyl-2Glc]$^-$, 459.3821 |

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| | | | [M-H-2Xyl-3Glc]$^-$ |
| $S_{PG}$-37*[C] | 16.97 | H [M-H-4Glc]$^-$ | 945.5386 [M-H-Glc]$^-$, 783.4864 [M-H-2Glc]$^-$, 621.4370 [M-H-3Glc]$^-$, 459.3810 [M-H-4Glc]$^-$ |
| $S_{PG}$-38 [m] | 17.32 | G/H [M-H-Ac-4Glc]$^-$ | 1107.5953 [M-H-Ac]$^-$, 1089.5863 [M-H-Ac-$H_2O$]$^-$, 945.5384 [M-H-Ac-Glc]$^-$, 783.4899 [M-H-Ac-2Glc]$^-$, 621.4239 [M-H-Ac-3Glc]$^-$, 459.3872 [M-H-Ac-4Glc]$^-$ |
| $S_{PG}$-39*[C] | 17.51 | I [M-H-2Glc-GlcA]$^-$ | 793.4382 [M-H-Glc]$^-$, 631.3800 [M-H-2Glc]$^-$, 455.3562 [M-H-2Glc-GlcA]$^-$ |
| $S_{PG}$-40*[C] | 17.51 | H [M-H-Xyl-3Glc]$^-$ | 945.5418 [M-H-Xyl]$^-$, 783.4890 [M-H-Xyl-Glc]$^-$, 621.4382 [M-H-Xyl-2Glc]$^-$, 459.3821 [M-H-Xyl-3Glc]$^-$ |
| $S_{PG}$-41[C] | 17.63 | G/H [M-H-2Xyl-3Glc]$^-$ | 1077.5848 [M-H-Xyl]$^-$, 945.5418 [M-H-2Xyl]$^-$, 783.4890 [M-H-2Xyl-Glc]$^-$, 621.4382 [M-H-2Xyl-2Glc]$^-$, 459.3821 [M-H-2Xyl-3Glc]$^-$ |
| $S_{PG}$-42[C] | 17.88 | G/H [M-H-Ac-Xyl-3Glc]$^-$ | 945.5452 [M-H-Ac-Xyl]$^-$, 927.5374 [M-H-Ac-Xyl-$H_2O$]$^-$, 783.4885 [M-H-Ac-Xyl-Glc]$^-$, 765.4813 [M-H-Ac-Xyl-Glc-$H_2O$]$^-$, 621.4388 [M-H-Ac-Xyl-2Glc]$^-$, 603.4418 [M-H-Ac-Xyl-2Glc-$H_2O$]$^-$, 459.3835 [M-H-Ac-Xyl-3Glc]$^-$, 375.2939 [M-H-Ac-Xyl-3Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-43*[C] | 18.09 | H [M-H-Xyl-3Glc]$^-$ | 945.5418 [M-H-Xyl]$^-$, 783.4890 [M-H-Xyl-Glc]$^-$, 621.4382 [M-H-Xyl-2Glc]$^-$, 459.3821 [M-H-Xyl-3Glc]$^-$ |
| $S_{PG}$-44*[C] | 18.28 | H [M-H-Xyl-3Glc]$^-$ | 945.5418 [M-H-Xyl]$^-$, 783.4890 [M-H-Xyl-Glc]$^-$, 621.4382 [M-H-Xyl-2Glc]$^-$, 459.3821 [M-H-Xyl-3Glc]$^-$ |
| $S_{PG}$-45[C] | 18.37 | G/H [M-H-Ac-Xyl-3Glc]$^-$ | 945.5452 [M-H-Ac-Xyl]$^-$, 927.5374 [M-H-Ac-Xyl-$H_2O$]$^-$, 783.4885 [M-H-Ac-Xyl-Glc]$^-$, 765.4813 [M-H-Ac-Xyl-Glc-$H_2O$]$^-$, 621.4388 [M-H-Ac-Xyl-2Glc]$^-$, 603.4418 [M-H-Ac-Xyl-2Glc-$H_2O$]$^-$, 459.3835 |

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| | | | [M-H-Ac-Xyl-3Glc]$^-$, 375.2939 [M-H-Ac-Xyl-3Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-46$^C$ | 18.74 | G/H [M-H-Ac-4Glc]$^-$ | 1107.5953 [M-H-Ac]$^-$, 1089.5863 [M-H-Ac-$H_2O$]$^-$, 945.5384 [M-H-Ac-Glc]$^-$, 783.4899 [M-H-Ac-2Glc]$^-$, 621.4239 [M-H-Ac-3Glc]$^-$, 459.3872 [M-H-Ac-4Glc]$^-$ |
| $S_{PG}$-47$^m$ | 19.1 | I [M-H-Glc-GlcA]$^-$ | 631.3884 [M-H-Glc]$^-$, 455.3487 [M-H-Glc-GlcA]$^-$ |
| $S_{PG}$-48*$^C$ | 19.23 | H [M-H-3Glc]$^-$ | 783.4855 [M-H-Glc]$^-$, 621.4365 [M-H-2Glc]$^-$, 459.3878 [M-H-3Glc]$^-$, 375.2877 [M-H-3Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-49$^C$ | 19.25 | G/H [M-H-Ac-Xyl-3Glc]$^-$ | 945.5452 [M-H-Ac-Xyl]$^-$, 927.5374 [M-H-Ac-Xyl-$H_2O$]$^-$, 783.4885 [M-H-Ac-Xyl-Glc]$^-$, 765.4813 [M-H-Ac-Xyl-Glc-$H_2O$]$^-$, 663.4493 [M-H-Xyl-2Glc]$^-$, 621.4388 [M-H-Ac-Xyl-2Glc]$^-$, 603.4418 [M-H-Ac-Xyl-2Glc-$H_2O$]$^-$, 459.3835 [M-H-Ac-Xyl-3Glc]$^-$, 375.2939 [M-H-Ac-Xyl-3Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-50$^m$ | 19.53 | G/H [M-H-Ac-3Glc]$^-$ | 783.4887 [M-H-Ac-Glc]$^-$, 621.4347 [M-H-Ac-2Glc]$^-$, 459.3852 [M-H-Ac-3Glc]$^-$ |
| $S_{PG}$-51$^m$ | 19.54 | G/H [M-H-Malonyl-3Glc]$^-$ | 945.5403 [M-H-Malonyl]$^-$, 783.4855 [M-H-Malonyl-Glc]$^-$, 621.4365 [M-H-Malonyl-2Glc]$^-$, 459.3878 [M-H-Malonyl-3Glc]$^-$, 375.2877 [M-H-Malonyl-3Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-52*$^C$ | 19.54 | G/H [M-H-3Glc]$^-$ | 783.4855 [M-H-Glc]$^-$, 621.4365 [M-H-2Glc]$^-$, 459.3878 [M-H-3Glc]$^-$, 375.2877 [M-H-3Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-53$^m$ | 19.73 | G/H [M-H-Ac-3Glc]$^-$ | 783.621.4347 [M-H-Ac-Glc]$^-$, 459.3852 [M-H-Ac-3Glc]$^-$ |
| $S_{PG}$-54$^C$ | 19.77 | G/H [M-H-3Glc]$^-$ | 783.4855 [M-H-Glc]$^-$, 621.4365 [M-H-2Glc]$^-$, 459.3878 [M-H-3Glc]$^-$, 375.2877 [M-H-3Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-55$^C$ | 19.79 | G/H [M-H-Ac-Xyl-3Glc]$^-$ | 945.5452 [M-H-Ac-Xyl]$^-$, 927.5374 [M-H-Ac-Xyl-$H_2O$]$^-$, 783.4885 [M-H-Ac-Xyl-Glc]$^-$, 765.4813 [M-H-Ac-Xyl-Glc-$H_2O$]$^-$, 663.4493 |

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| | | | [M-H-Xyl-2Glc]$^-$, 621.4388 [M-H-Ac-Xyl-2Glc]$^-$, 603.4418 [M-H-Ac-Xyl-2Glc-$H_2O$]$^-$, 459.3835 [M-H-Ac-Xyl-3Glc]$^-$, 375.2939 [M-H-Ac-Xyl-3Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-56$^C$ | 20.17 | G/H [M-H-3Glc]$^-$ | 783.4855 [M-H-Glc]$^-$, 621.4365 [M-H-2Glc]$^-$, 459.3878 [M-H-3Glc]$^-$, 375.2877 [M-H-3Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-57$^C$ | 20.35 | G/H [M-H-Ac-3Glc]$^-$ | 783.4849 [M-H-Ac-Glc]$^-$, 621.4347 [M-H-Ac-2Glc]$^-$, 459.3852 [M-H-Ac-3Glc]$^-$ |
| $S_{PG}$-58 $^m$ | 20.75 | G/H [M-H-Xyl-2Glc]$^-$ | 783.4897 [M-H-Xyl]$^-$, 765.4748 [M-H-Xyl-$H_2O$]$^-$, 621.4368 [M-H-Xyl-Glc]$^-$, 459.3809 [M-H-Xyl-2Glc]$^-$, 375.2876 [M-H-Xyl-2Glc-$C_6H_{12}$]$^-$ |
| $S_{PG}$-59$^C$ | 21.19 | G/H [M-H-Ac-3Glc]$^-$ | 783.621.4347 [M-H-Ac-Glc]$^-$, 459.3852 [M-H-Ac-3Glc]$^-$ |
| $S_{PG}$-60 $^m$ | 21.25 | D/E/F [M-H-Xyl-Glc]$^-$ | 619.4210 [M-H-Xyl]$^-$, 457.3684 [M-H-Xyl-Glc]$^-$ |
| $S_{PG}$-61 $^m$ | 21.75 | D/E/F [M-H-Xyl-Glc]$^-$ | 619.4210 [M-H-Xyl]$^-$, 457.3684 [M-H-Xyl-Glc]$^-$ |
| $S_{PG}$-62*$^C$ | 21.79 | F [M-H-Rha-Glc]$^-$ | 619.4276 [M-H-Rha]$^-$, 457.3452 [M-H-Rha-Glc]$^-$ |
| $S_{PG}$-63*$^C$ | 22.27 | E [M-H-Rha-Glc]$^-$ | 619.4276 [M-H-Rha]$^-$, 457.3452 [M-H-Rha-Glc]$^-$ |
| $S_{PG}$-64$^C$ | 23.04 | G/H [M-H-2Glc]$^-$ | 621.4338 [M-H-Glc]$^-$, 459.3880 [M-H-2Glc]$^-$ |
| $S_{PG}$-65 $^m$ | 23.5 | I [M-H-Glc-GlcA]$^-$ | 631.3884 [M-H-Glc]$^-$, 455.3487 [M-H-Glc-GlcA]$^-$ |
| $S_{PG}$-66*$^C$ | 24.4 | H [M-H-2Glc]$^-$ | 621.4338 [M-H-Glc]$^-$, 459.3880 [M-H-2Glc]$^-$ |
| $S_{PG}$-67$^C$ | 24.72 | G/H [M-H-2Glc]$^-$ | 621.4338 [M-H-Glc]$^-$, 459.3880 [M-H-2Glc]$^-$ |
| $S_{PG}$-68*$^C$ | 27.55 | C [M-H-2Glc]$^-$ | 603.3776 [M-H-Glc]$^-$, 441.3452 [M-H-2Glc]$^-$ |
| $S_{PG}$-69*$^C$ | 27.88 | A [M-H-2Glc]$^-$ | 603.3776 [M-H-Glc]$^-$, 441.3452 [M-H-2Glc]$^-$ |
| $S_{PG}$-70 $^m$ | 28 | A/B/C [M-H-Ac-2Glc]$^-$ | 765.4600 [M-H-Ac]$^-$, 603.3768 [M-H-Ac-Glc]$^-$, 441.2103 [M-H-Ac-2Glc]$^-$ |
| $S_{PG}$-71 $^m$ | 28.2 | G/H [M-H-Glc]$^-$ | 459.3880 [M-H-Glc]$^-$ |
| $S_{PG}$-72 $^m$ | 28.41 | G/H [M-H-Glc]$^-$ | 459.3880 [M-H-Glc]$^-$ |
| $S_{PG}$-73 $^m$ | 29.57 | A/B/C [M-H-Ac-2Glc]$^-$ | 765.4600 [M-H-Ac]$^-$, 603.3768 |

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| | | | [M-H-Ac-Glc]$^-$, 441.2103 [M-H-Ac-2Glc]$^-$ |
| $F_{AM}$-8 [m] | 6.4 | FA-2 [M-H-2Glc]$^-$ | 433.1382 [M-H-Glc]$^-$, 271.0624 [M-H-2Glc]$^-$, 151.0033 [M-H-2Glc-$C_8H_8O$]$^-$, 119.0527 [M-H-2Glc-$C_7H_4O_4$]$^-$ |
| $F_{AM}$-13[C] | 7.46 | FA-10 [M-H-Glc]$^-$ | 299.0550 [M-H-Glc]$^-$, 284.0317 [M-H-Glc]$^-$, 135.0079 [M-H-Glc-$C_9H_8O_3$]$^-$ |
| $F_{AM}$-36 [m] | 10 | FA-12 [M-H-Api-Glc]$^-$ | 463.1601 [M-H-Api]$^-$, 301.0707 [M-H-Api-Glc]$^-$ |
| $F_{AM}$-38 [m] | 10.82 | FA-5 [M-H-Glc]$^-$ | 269.0446 [M-H-Glc]$^-$ |
| $F_{AM}$-40 [m] | 11.21 | FA-10 [M-H-Glc]$^-$ | 299.0550 [M-H-Glc]$^-$, 284.0317 [M-H-Glc-$CH_3$]$^-$, 135.0079 [M-H-Glc-$CH_3$-$C_8H_5O_3$]$^-$ |
| $F_{AM}$-41 [m] | 11.25 | FA-7 [M-H-Glc]$^-$ | 283.0610 [M-H-Glc]$^-$, 268.0359 [M-H-Glc-$CH_3$]$^-$ |
| $F_{AM}$-43 [m] | 11.44 | FA-12 [M-H-2Glc]$^-$ | 463.1591 [M-H-Glc]$^-$, 301.0704 [M-H-2Glc]$^-$, 271.0627 [M-H-2Glc-$2CH_3$]$^-$ |
| $F_{AM}$-47 [m] | 11.6 | FA-8 [M-H-Glc]$^-$ | 285.0752 [M-H-Glc]$^-$ |
| $F_{AM}$-49 [m] | 12.1 | FA-12 [M-H-Glc]$^-$ | 301.1099 [M-H-Glc]$^-$, 271.0624 [M-H-Glc-$2CH_3$]$^-$ |
| $F_{AM}$-50 [m] | 12.28 | FA-12 [M-H-Api]$^-$ | 403.1396 [M-H-$CH_2O$]$^-$, 373.1224 [M-H-$2CH_2O$]$^-$, 301.1099 [M-H-Api]$^-$, 283.0561 [M-H-Api-$H_2O$]$^-$ |
| $F_{AM}$-54 [m] | 12.8 | FA-3 [M-H]$^-$ | 135.0085 [M-H-$C_8H_6O$]$^-$ |
| $F_{AM}$-60 [m] | 13.3 | FA-12 [M-H-Glc]$^-$ | 301.1099 [M-H-Glc]$^-$, 271.0624 [M-H-Glc-$CH_3$]$^-$ |
| $F_{AM}$-62 [m] | 13.6 | FA-7 [M-H]$^-$ | 283.0607 [M-H]$^-$, 268.0450 [M-H-$CH_3$]$^-$ |
| $F_{AM}$-64* [m] | 13.7 | FA-3 [M-H]$^-$ | 135.0085 [M-H-$C_8H_6O$]$^-$ |
| $F_{AM}$-67 [m] | 13.91 | FA-4 [M-H-Acetyl-Glc]$^-$ | 267.1 [M-H-Acetyl-Glc]$^-$, 252.0420 [M-H-Acetyl-Glc-$CH_3$]$^-$, 135.0101 [M-H-Acetyl-Glc-$CH_3$-$C_8H_5O$]$^-$ |
| $F_{AM}$-68 [m] | 14.2 | FA-7 [M-H]$^-$ | 268.0450 [M-H-$CH_3$]$^-$ |
| $F_{AM}$-69 [m] | 14.22 | FA-1 [M-H-2Glc]$^-$ | 255.0657 [M-H-2Glc]$^-$, 135.0081 [M-H-2Glc-$C_8H_8O$]$^-$, 119.0495 [M-H-2Glc-$C_7H_4O_3$]$^-$ |
| $F_{AM}$-70 [m] | 14.23 | FA-11 [M-H-Api-Glc]$^-$ | 299.0897 [M-H-Api-Glc]$^-$, 284.0686 [M-H-Api-Glc-$CH_3$]$^-$, 269.0417 [M-H-Api-Glc-$2CH_3$]$^-$ |
| $F_{AM}$-71 [m] | 14.47 | FA-11 [M-H-Api-Glc]$^-$ | 299.0897 [M-H-Api-Glc]$^-$, 284.0686 [M-H-Api-Glc-$CH_3$]$^-$, 269.0417 [M-H-Api-Glc-$2CH_3$]$^-$ |
| $F_{AM}$-72[C] | 15.07 | FA-12 [M-H-Glc]$^-$ | 301.1099 [M-H-Glc]$^-$, 271.0624 |

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| | | | [M-H-Glc-2$CH_3$]$^-$ |
| $F_{AM}$-75*[C] | 15.22 | FA-7 [M-H]$^-$ | 135.0081 [M-H-$C_8H_8O$]$^-$, 119.0495 [M-H-$C_7H_4O_3$]$^-$ |
| $F_{AM}$-76*[C] | 15.7 | FA-12 [M-H-Glc]$^-$ | 301.1099 [M-H-Glc]$^-$, 271.0624 [M-H-Glc-2$CH_3$]$^-$ |
| $F_{AM}$-77 [m] | 17.87 | FA-5 [M-H]$^-$ | 133.0286 [M-H-$C_7H_3O_3$]$^-$ |
| $F_{AM}$-78 [m] | 18.3 | FA-10 [M-H]$^-$ | 284.0305 [M-H-$CH_3$]$^-$, 269.0441 [M-H-2$CH_3$]$^-$ |
| $F_{AM}$-79 [m] | 18.9 | FA-11 [M-H]$^-$ | 284.0682 [M-H-$CH_3$]$^-$, 269.0434 [M-H-2$CH_3$]$^-$ |
| $F_{AM}$-80 [m] | 19.01 | FA-11 [M-H]$^-$ | 284.0682 [M-H-$CH_3$]$^-$, 269.0434 [M-H-2$CH_3$]$^-$ |
| $F_{AM}$-81[C] | 19.09 | FA-3 [M-H]$^-$ | 135.0085 [M-H-$C_8H_6O$]$^-$ |
| $F_{AM}$-82*[C] | 20.25 | FA-4 [M-H]$^-$ | 252.0419 [M-H-$CH_3$]$^-$ |
| $F_{CC}$-3[C] | 4.97 | FA-9 [M-H]$^-$ | 137.0238 [M-H-$C_8H_8O_3$]$^-$, 109.0296 [M-H-$C_9H_8O_4$]$^-$ |
| $F_{CC}$-9[C] | 6.65 | FA-9 [M-H]$^-$ | 137.0238 [M-H-$C_8H_8O_3$]$^-$, 109.0296 [M-H-$C_9H_8O_4$]$^-$ |
| $F_{CC}$-11 [m] | 6.69 | FA-9 [M-H]$^-$ | 137.0238 [M-H-$C_8H_8O_3$]$^-$, 109.0296 [M-H-$C_9H_8O_4$]$^-$ |
| $F_{GU,AM}$-25*[C] | 8.95 | FA-7 [M-H-Glc]$^-$ | 283.0607 [M-H-Glc]$^-$, 268.0450 [M-H-Glc-$CH_3$]$^-$ |
| $F_{GU,AM}$-51 [m] | 12.3 | FA-4 [M-H-Api-Glc]$^-$ | 267.0661 [M-H-Api-Glc]$^-$, 252.0420 [M-H-Api-Glc-$CH_3$]$^-$, 135.0101 [M-H-Api-Glc-$CH_3$-$C_8H_5O$]$^-$ |
| $F_{GU,AM}$-55 [m] | 13 | FA-4 [M-H-Api-Glc]$^-$ | 267.0661 [M-H-Api-Glc]$^-$, 252.0420 [M-H-Api-Glc-$CH_3$]$^-$, 135.0101 [M-H-Api-Glc-$CH_3$-$C_8H_5O$]$^-$ |
| $F_{GU}$-2 [m] | 3.95 | FA-1 [M-H-$C_4H_2O_2$-2Glc]$^-$ | 579.1732 [M-H-$C_4H_2O_2$]$^-$, 417.1187 [M-H-$C_4H_2O_2$-Glc]$^-$, 255.0657 [M-H-$C_4H_2O_2$-2Glc]$^-$, 135.0081 [M-H-$C_4H_2O_2$-2Glc-$C_8H_8O$]$^-$, 119.0495 [M-H-$C_4H_2O_2$-2Glc-$C_7H_4O_3$]$^-$ |
| $F_{GU}$-4 [m] | 5.7 | FA-1 [M-H-$C_4H_2O_2$-Glc]$^-$ | 417.1187 [M-H-$C_4H_2O_2$]$^-$, 255.0657 [M-H-$C_4H_2O_2$-Glc]$^-$, 135.0081 [M-H-$C_4H_2O_2$-Glc-$C_8H_8O$]$^-$,119.0495 [M-H-$C_4H_2O_2$-Glc-$C_7H_4O_3$]$^-$ |
| $F_{GU}$-5 [m] | 5.87 | FA-1 [M-H-$C_4H_2O_2$-Glc]$^-$ | 417.1187 [M-H-$C_4H_2O_2$]$^-$, 255.0657 [M-H-$C_4H_2O_2$-Glc]$^-$, 135.0081 [M-H-$C_4H_2O_2$-Glc-$C_8H_8O$]$^-$, 119.0495 [M-H-$C_4H_2O_2$-Glc-$C_7H_4O_3$]$^-$ |
| $F_{GU}$-6 [m] | 5.88 | FA-1 [M-H-$C_4H_2O_2$-Api-Glc]$^-$ | 549.1642 [M-H-$C_4H_2O_2$]$^-$, 417.1187 [M-H-$C_4H_2O_2$-Api]$^-$, 255.0657 [M-H-$C_4H_2O_2$-Api-Glc]$^-$, 135.0081 |

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|---|---|---|---|
| | | | [M-H-$C_4H_2O_2$-Api-Glc-$C_8H_8O$]$^-$, 119.0495 [M-H-$C_4H_2O_2$-Api-Glc-$C_7H_4O_3$]$^-$ |
| $F_{GU}$-7$^C$ | 6.18 | FA-1 [M-H-2Glc]$^-$ | 417.1187 [M-H-Glc]$^-$, 255.0657 [M-H-2Glc]$^-$, 135.0081 [M-H-2Glc-$C_8H_8O$]$^-$, 119.0495 [M-H-2Glc-$C_7H_4O_3$]$^-$ |
| $F_{GU}$-10$^m$ | 6.65 | FA-1 [M-H-Api-2Glc]$^-$ | 549.1641 [M-H-Glc]$^-$, 417.1187 [M-H-Api-Glc]$^-$, 255.0657 [M-H-Api-2Glc]$^-$, 135.0081 [M-H-Api-2Glc-$C_8H_8O$]$^-$, 119.0495 [M-H-Api-2Glc-$C_7H_4O_3$]$^-$ |
| $F_{GU}$-12$^C$ | 7.21 | FA-5 [M-H-2Glc]$^-$ | 473.1127 [M-H-$C_4H_8O_4$]$^-$, 383.0768 [M-H-$C_4H_8O_4$-$C_3H_6O_3$]$^-$, 353.0674 [M-H-2$C_4H_8O_4$]$^-$, 325.0608 [M-H-2$C_4H_8O_4$-CO]$^-$ |
| $F_{GU}$-14$^m$ | 7.66 | FA-3 [M-H-Glc]$^-$ | 253.0512 [M-H-Glc]$^-$, 135.0110 [M-H-Glc-$C_8H_6O$]$^-$ |
| $F_{GU}$-15$^m$ | 7.7 | FA-2 [M-H-2Glc]$^-$ | 433.1127 [M-H-Glc]$^-$, 271.0624 [M-H-2Glc]$^-$, 151.0033 [M-H-2Glc-$C_8H_8O$]$^-$, 119.0527 [M-H-2Glc-$C_7H_4O_4$]$^-$ |
| $F_{GU}$-16$^C$ | 8.1 | FA-5 [M-H-Glc-Api]$^-$ | 503.1192 [M-H-$C_2H_4O_2$]$^-$, 443.098 [M-H-$C_4H_8O_4$]$^-$, 353.0674 [M-H-$C_4H_8O_4$-$C_3H_6O_3$]$^-$ |
| $F_{GU}$-17$^C$ | 8.2 | FA-1 [M-H-2Glc]$^-$ | 255.0657 [M-H-2Glc]$^-$, 135.0081 [M-H-2Glc-$C_8H_8O$]$^-$, 119.0495 [M-H-2Glc-$C_7H_4O_3$]$^-$ |
| $F_{GU}$-18$^m$ | 8.34 | FA-1 [M-H-Api-2Glc]$^-$ | 549.1609 [M-H-Glc]$^-$, 417.1187 [M-H-Api-Glc]$^-$, 255.0657 [M-H-Api-2Glc]$^-$, 135.0081 [M-H-Api-2Glc-$C_8H_8O$]$^-$, 119.0495 [M-H-Api-2Glc-$C_7H_4O_3$]$^-$ |
| $F_{GU}$-19$^m$ | 8.41 | FA-3 [M-H-Glc]$^-$ | 253.0512 [M-H-Glc]$^-$, 135.0110 [M-H-Glc-$C_8H_6O$] |
| $F_{GU}$-20$^m$ | 8.42 | FA-3 [M-H-Glc-Api]$^-$ | 415.1027 [M-H-Api]$^-$, 253.0512 [M-H-Glc-Api]$^-$, 135.0110 [M-H-Glc-Api-$C_8H_6O$]$^-$ |
| $F_{GU}$-21$^m$ | 8.64 | FA-1 [M-H-Api-2Glc]$^-$ | 549.1609 [M-H-Glc]$^-$, 417.1187 [M-H-Api-Glc]$^-$, 255.0657 [M-H-Api-2Glc]$^-$, 135.0081 [M-H-Api-2Glc-$C_8H_8O$]$^-$, 119.0495 [M-H-Api-2Glc-$C_7H_4O_3$]$^-$ |

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| $F_{GU}$-22 [m] | 8.75 | FA-3 [M-H-Glc-Api]$^-$ | 415.1027 [M-H-Api]$^-$, 253.0512 [M-H-Glc-Api]$^-$, 135.0110 [M-H-Glc-Api-$C_8H_6O$]$^-$ |
| $F_{GU}$-23[C] | 8.75 | FA-2 [M-H-Glc]$^-$ | 271.0606 [M-H-Glc]$^-$ |
| $F_{GU}$-24[C] | 8.82 | FA-1 [M-H-2Glc]$^-$ | 255.0657 [M-H-2Glc]$^-$, 135.0081 [M-H-2Glc-$C_8H_8O$]$^-$, 119.0495 [M-H-2Glc-$C_7H_4O_3$]$^-$ |
| $F_{GU}$-26[C] | 8.96 | FA-1 [M-H-Glc]$^-$ | 255.0668 [M-H-Glc]$^-$, 135.0092 [M-H-Glc-$C_8H_8O$]$^-$ |
| $F_{GU}$-27[C] | 9 | FA-1 [M-H-2Glc]$^-$ | 417.1216 [M-H-2Glc]$^-$, 255.0657 [M-H-2Glc]$^-$, 135.0081 [M-H-2Glc-$C_8H_8O$]$^-$, 119.0495 [M-H-2Glc-$C_7H_4O_3$]$^-$ |
| $F_{GU}$-28 [m] | 9.01 | FA-2 [M-H-Glc]$^-$ | 271.0624 [M-H-Glc]$^-$, 151.0033 [M-H-Glc-$C_8H_8O$]$^-$, 119.0527 [M-H-Glc-$C_7H_4O_4$]$^-$ |
| $F_{GU}$-29[C] | 9.02 | FA-1 [M-H-Api-Glc]$^-$ | 417.1216 [M-H-Api-Glc]$^-$, 255.0657 [M-H-Api-Glc]$^-$, 135.0081 [M-H-Api-Glc-$C_8H_8O$]$^-$, 119.0495 [M-H-Api-Glc-$C_7H_4O_3$]$^-$ |
| $F_{GU}$-30*[C] | 9.11 | FA-1 [M-H-Glc]$^-$ | 255.0657 [M-H-Glc]$^-$, 135.0081 [M-H-Glc-$C_8H_8O$]$^-$, 119.0495 [M-H-Glc-$C_7H_4O_3$]$^-$ |
| $F_{GU}$-31*[C] | 9.4 | FA-1 [M-H-Api-Glc]$^-$ | 417.1216 [M-H-Api-Glc]$^-$, 255.0657 [M-H-Api-Glc]$^-$, 135.0081 [M-H-Api-Glc-$C_8H_8O$]$^-$, 119.0495 [M-H-Api-Glc-$C_7H_4O_3$]$^-$ |
| $F_{GU}$-32 [m] | 9.51 | FA-8 [M-H-Glc]$^-$ | 285.0695 [M-H-Glc]$^-$ |
| $F_{GU}$-33[C] | 9.61 | FA-5 [M-H-Rha-Glc]$^-$ | 473.1083 [M-H-$C_4H_8O_3$]$^-$, 457.1123 [M-H-$C_4H_8O_4$]$^-$, 383.0755 [M-H-$C_4H_8O_3$-$C_3H_6O_3$]$^-$, 353.0664 [M-H-$C_4H_8O_3$-$C_4H_8O_4$]$^-$ |
| $F_{GU}$-34 [m] | 9.7 | FA-2 [M-H-Api-Glc]$^-$ | 433.1127 [M-H-Api]$^-$, 271.0609 [M-H-Api-Glc]$^-$, 243.0657 [M-H-Api-Glc-CO]$^-$ |
| $F_{GU}$-35 [m] | 9.7 | FA-8 [M-H-Glc]$^-$ | 285.0695 [M-H-Glc]$^-$ |
| $F_{GU}$-37 [m] | 10.6 | FA-1 [M-H-Glc]$^-$ | 255.0657 [M-H-Glc]$^-$, 135.0081 [M-H-Api-Glc-$C_8H_8O$]$^-$, 119.0495 [M-H-Api-Glc-$C_7H_4O_3$]$^-$ |
| $F_{GU}$-39 [m] | 11 | FA-8 [M-H-Glc]$^-$ | 285.0695 [M-H-Glc]$^-$ |
| $F_{GU}$-42 [m] | 11.25 | FA-8 [M-H-Glc]$^-$ | 285.0695 [M-H-Glc]$^-$ |
| $F_{GU}$-44 [m] | 11.48 | FA-2 [M-H-Api-Glc]$^-$ | 433.1127 [M-H-Api]$^-$, 271.0624 [M-H-Api-Glc]$^-$, 151.0033 [M-H-Api-Glc-$C_8H_8O$]$^-$ |

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| $F_{GU}$-45[C] | 11.48 | FA-2 $[M-H-Glc]^-$ | 271.0624 $[M-H-Glc]^-$, 151.0033 $[M-H-Glc-C_8H_8O]^-$ |
| $F_{GU}$-46[m] | 11.5 | FA-1 $[M-H-2Glc]^-$ | 417.1216 $[M-H-2Glc]^-$, 255.0657 $[M-H-2Glc]^-$, 135.0081 $[M-H-2Glc-C_8H_8O]^-$, 119.0495 $[M-H-2Glc-C_7H_4O_3]^-$ |
| $F_{GU}$-48[m] | 11.9 | FA-1 $[M-H-Api-Glc]^-$ | 417.1216 $[M-H-Api]^-$, 255.0657 $[M-H-Api-Glc]^-$, 135.0081 $[M-H-Api-Glc-C_8H_8O]^-$, 119.0495 $[M-H-Api-Glc-C_7H_4O_3]^-$ |
| $F_{GU}$-52[m] | 12.4 | FA-6 $[M-H-Glc]^-$ | 269.0819 $[M-H-Glc]^-$ |
| $F_{GU}$-53[m] | 12.75 | FA-7 $[M-H-Glc]^-$ | 283.0610 $[M-H-Glc]^-$, 268.0359 $[M-H-Glc-CH_3]^-$, 135.0110 $[M-H-Glc-CH_3-C_8H_5O_2]^-$ |
| $F_{GU}$-56[m] | 13 | FA-1 $[M-H-2Glc]^-$ | 255.0657 $[M-H-2Glc]^-$, 135.0081 $[M-H-2Glc-C_8H_8O]^-$, 119.0495 $[M-H-2Glc-C_7H_4O_3]^-$ |
| $F_{GU}$-57*[C] | 13.1 | FA-4 $[M-H-Glc]^-$ | 267.0621 $[M-H-Glc]^-$, 252.0420 $[M-H-Glc-CH_3]^-$, 135.0101 $[M-H-Glc-CH_3-C_8H_5O]^-$ |
| $F_{GU}$-58[m] | 13.1 | FA-1 $[M-H-Ac-2Glc]^-$ | 549.1609 $[M-H-Ac]^-$, 417.1216 $[M-H-Ac-Glc]^-$, 255.0657 $[M-H-Ac-2Glc]^-$, 135.0081 $[M-H-Ac-2Glc-C_8H_8O]^-$, 119.0495 $[M-H-Ac-2Glc-C_7H_4O_3]^-$ |
| $F_{GU}$-59*[C] | 13.21 | FA-1 $[M-H-Api-Glc]^-$ | 417.1216 $[M-H-Glc]^-$, 255.0657 $[M-H-Api-Glc]^-$, 135.0081 $[M-H-Api-Glc-C_8H_8O]^-$, 119.0495 $[M-H-Api-Glc-C_7H_4O_3]^-$ |
| $F_{GU}$-61[C] | 13.5 | FA-1 $[M-H-Glc]^-$ | 255.0657 $[M-H-Glc]^-$, 135.0081 $[M-H-Glc-C_8H_8O]^-$, 119.0495 $[M-H-Glc-C_7H_4O_3]^-$ |
| $F_{GU}$-63[m] | 13.63 | FA-1 $[M-H-Ac-Glc]^-$ | 417.1187 $[M-H-Ac]^-$, 255.0650 $[M-H-Ac-Glc]^-$, 135.0077 $[M-H-Ac-Glc-C_8H_8O]^-$ |
| $F_{GU}$-65*[C] | 13.81 | FA-1 $[M-H-Api-Glc]^-$ | 417.1216 $[M-H-Api]^-$, 255.0657$[M-H-Api-Glc]^-$, 135.0081 $[M-H-Api-Glc-C_8H_8O]^-$, 119.0495 $[M-H-Api-Glc-C_7H_4O_3]^-$ |
| $F_{GU}$-66*[C] | 13.9 | FA-1 $[M-H]^-$ | 135.0081 $[M-H-C_8H_8O]^-$, 119.0495 $[M-H-C_7H_4O_3]^-$ |
| $F_{GU}$-73[m] | 15.13 | FA-2 $[M-H-Glc]^-$ | 271.0624 $[M-H-Glc]^-$, 151.0033 $[M-H-Glc-C_8H_8O]^-$ |

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| $F_{GU}$-74 [m] | 15.2 | FA-1 [M-H-Rha-Api-Glc]$^-$ | 417.1216 [M-H-Api]$^-$, 255.0657[M-H-Api-Glc]$^-$, 135.0081 [M-H-Api-Glc-$C_8H_8O$]$^-$, 119.0495 [M-H-Api-Glc-$C_7H_4O_3$]$^-$ |
| $F_{GU}$-79 [m] | 18.56 | FA-1 [M-H-Ac-Glc]$^-$ | 417.1557 [M-H-Ac]$^-$, 255.065055.1 [M-H-Ac-Glc]$^-$,135.0077 [M-H Ac-Glc-$C_8H_8O$]$^-$ |
| $F_{GU}$-83*[C] | 20.26 | FA-1 [M-H]$^-$ | 135.0080 [M-H-$C_8H_8O$]$^-$,119.0493 [M-H-$C_7H_4O_3$]$^-$ |
| $P_{CC}$-1[C] | 4.98 | FA-9 | 425.087 [M-H-$C_8H_8O_3$]$^-$,289.071 [M-H-$C_{15}H_{13}O_6$]$^-$ |
| $P_{CC}$-2[C] | 5.73 | FA-9 | 425.087 [M-H-$C_8H_8O_3$]$^-$,289.071 [M-H-$C_{15}H_{13}O_6$]$^-$ |
| $P_{CC}$-3[C] | 6.14 | FA-9 | 425.087 [M-H-$C_8H_8O_3$]$^-$,289.071 [M-H-$C_{15}H_{13}O_6$]$^-$ |
| $P_{CC}$-4[C] | 6.54 | FA-9 | 425.087 [M-H-$C_8H_8O_3$]$^-$,289.071 [M-H-$C_{15}H_{13}O_6$]$^-$ |
| $P_{CC}$-5[C] | 9.27 | FA-9 | 425.087 [M-H-$C_8H_8O_3$]$^-$,289.071 [M-H-$C_{15}H_{13}O_6$]$^-$ |
| $P_{CC}$-6[C] | 10.46 | FA-9 | 713.151 [M-H-$C_8H_8O_3$]$^-$,577.135 [M-H-$C_{15}H_{13}O_6$]$^-$,425.087 [M-H-$C_{15}H_{13}O_6$-$C_8H_8O_3$]-,289.071 [M-H-$C_{15}H_{13}O_6$]$^-$ |
| $L_{CC}$-1[C] | 10.02 | | 521.202 [M-H-Api]$^-$,359.149 [M-H-Api-Glc]$^-$,341.139 [M-H-Api-Glc-$H_2O$]$^-$,326.115 [M-H-Api-Glc-$H_2O$-$CH_3$]$^-$ |
| $L_{CC}$-2[C] | 10.05 | | 521.202 [M-H-Api]$^-$,359.149 [M-H-Api-Glc]$^-$,341.139 [M-H-Api-Glc-$H_2O$]$^-$,326.115 [M-H-Api-Glc-$H_2O$-$CH_3$]$^-$ |
| $L_{CC}$-3[C] | 10.29 | | 389.159 [M-H-Glc]$^-$,371.149 [M-H-Glc-$H_2O$]$^-$,341.105 [M-H-Glc-$H_2O$-2$CH_3$]$^-$ |
| $L_{CC}$-4[C] | 10.39 | | 359.149 [M-H-Glc]$^-$,341.139 [M-H-Glc-$H_2O$]$^-$,326.115 [M-H-Glc-$H_2O$-$CH_3$]$^-$ |
| $D_{CC}$-1[C] | 3.04 | | 381.1913 [M-H-Glc]$^-$ |
| $D_{CC}$-2*[C] | 6.05 | | 347.1857 [M-H-$H_2O$]$^-$ |
| $D_{CC}$-3*[C] | 6.51 | | 407.2070 [M-H-$H_2O$]$^-$ |
| $D_{CC}$-4*[C] | 14.4 | | 389.1964 [M-H-$H_2O$]$^-$ |

**Notes,** *: the compound identified by comparison with the reference.

[C]: the compound identified by UNIFI.

[m]: the compound detected by the multiple screening modes of Qtrap-MS.

F: flavonoid; S:saponin; P: procyanidin; L: lignan; D: diterpene.

[AM]: the compound originated from *A. membranceus*; [GU]: the compound originated from *G. uralensis*; [PG]: the compound originated from *P. ginseng*; and [CC]: the compound originated from *C. cassia*.

**Table S2 The ion transitions, corresponding $t_R$, and optimal DPs and CEs for 175 quantitated and semi-quantitated compounds.**

| Analyte | $t_R$ (min) | Ion transition (*m/z*) | DP (V) | CE (eV) |
|---|---|---|---|---|
| Re1/Re2/Re3/20-glu-Rf/NotoginsenosideM/N/Vinaginsenoside R4 | 3.61 | 1007 > 961 | -200 | -33 |
| Q-*O*-Glc-Glc-Glc | 2.79 | 1025 > 979 | -200 | -33 |
| Apigenin-6,8-di-*C*-*β*-D-glucopyranoside* | 3.43 | 593 > 473 | -150 | -38 |
| Re1/Re2/Re3/20-glu-Rf/NotoginsenosideM/N/Vinaginsenoside R4 | 3.65 | 1007 > 961 | -200 | -33 |
| Neoliquiritin apioside | 4.02 | 549 > 255 | -164 | -41 |
| Isomer of liquiritin apioside | 4.40 | 549 > 255 | -164 | -41 |
| Calycosin-7-*O*-*β*-D-glucoside* | 4.64 | 445 > 283 | -84 | -22 |
| Liquiritin* | 4.67 | 417 > 255 | -101 | -30 |
| Liquiritin apioside* | 4.77 | 549 > 255 | -164 | -41 |
| Catechin or epicatechin | 4.97 | 289 > 245 | -125 | -25 |
| PAC B-type dimer | 4.98 | 577 > 407 | -135 | -25 |
| Gypenoside Gc7 | 5.22 | 1007 > 961 | -200 | -33 |
| PAC B-type dimer | 5.73 | 577 > 407 | -135 | -25 |
| PAC B-type dimer | 6.14 | 577 > 407 | -135 | -25 |
| Isomer of liquiritigenin-*O*-diglucoside | 6.18 | 579 > 255 | -135 | -25 |
| PAC B-type dimer | 6.54 | 577 > 407 | -135 | -25 |
| Isomer of calycosin | 6.60 | 283 > 268 | -90 | -27 |
| Catechin or Epicatechin | 6.65 | 289 > 245 | -125 | -25 |
| Catechin or Epicatechin | 6.69 | 289 > 245 | -125 | -25 |
| Re1/Re2/Re3/20-glu-Rf/NotoginsenosideM/N/Vinaginsenoside R4 | 7.02 | 1007 > 961 | -200 | -33 |
| Isoliquiritin apioside* | 7.06 | 549 > 255 | -164 | -41 |
| Ginsenoside Rg1* | 7.10 | 845 > 799 | -150 | -33 |
| Ginsenoside Re* | 7.15 | 991 > 945 | -200 | -33 |
| Isoliquiritin* | 7.17 | 417 > 255 | -101 | -30 |
| Isomer of calycosin, | 7.20 | 283 > 268 | -90 | -27 |
| Liquiritigenin* | 7.26 | 255 > 135 | -80 | -24 |
| Ginsenoside Rf2 | 7.27 | 847 > 801 | -150 | -33 |
| Ononin* | 7.28 | 475 > 267 | -100 | -21 |
| Isomer of ginsenoside Rg1 | 7.40 | 845 > 799 | -150 | -33 |
| Isomer of 5'-hydroxy-4'-methoxyisoflavone-3'-*β*-D-glucoside | 7.46 | 461 > 299 | -125 | -25 |
| Re4/Notoginsenoside R1 | 7.71 | 977 > 931 | -150 | -33 |
| Re1/Re2/Re3/20-glu-Rf/NotoginsenosideM/N/Vinaginsenoside R4 | 7.74 | 1007 > 961 | -200 | -33 |
| Isomer of ginsenoside Rg1 | 7.80 | 845 > 799 | -150 | -33 |
| Licuraside | 7.81 | 549 > 255 | -164 | -41 |
| Calycosin* | 8.11 | 283 > 268 | -90 | -27 |
| Isomer of ginsenoside Rg1 | 8.12 | 845 > 799 | -150 | -33 |
| Uralsaponin C* | 8.19 | 823 > 351 | -185 | -58 |
| Liquiritigenin-*O*-diglucoside | 8.20 | 579 > 255 | -135 | -25 |

| | | | | |
|---|---|---|---|---|
| Re4/Notoginsenoside R1 | 8.39 | 977 > 931 | -150 | -33 |
| Yunganoside G2 | 8.44 | 839 > 351 | -185 | -58 |
| Floralginsenoside C | 8.56 | 847 > 801 | -150 | -33 |
| 5-Hydroxy-liquiritin or 8-Hydroxy-liquiritin | 8.75 | 433 > 271 | -135 | -25 |
| Liquiritigenin-*O*-diglucoside | 8.82 | 579 > 255 | -135 | -25 |
| Uralsaponin F* | 8.88 | 895 > 351 | -185 | -58 |
| Re1/Re2/Re3/20-glu-Rf/NotoginsenosideM/N/Vinaginsenoside R4 | 8.90 | 1007 > 961 | -200 | -33 |
| g-*O*-Rha-GlcA-GlcA | 8.90 | 969 > 351 | -185 | -58 |
| Neoliquiritin | 8.96 | 417 > 255 | -101 | -30 |
| Liquiritigenin-*O*-diglucoside | 9.00 | 579 > 255 | -135 | -25 |
| Re1/Re2/Re3/20-glu-Rf/NotoginsenosideM/N/Vinaginsenoside R4 | 9.01 | 1007 > 961 | -200 | -33 |
| 5-Hydroxy-liquiritin or 8-Hydroxy-liquiritin | 9.01 | 433 > 271 | -135 | -25 |
| Isomer of uralsaponin F | 9.22 | 895 > 351 | -185 | -58 |
| PAC B-type dimer | 9.27 | 577 > 407 | -135 | -25 |
| Licorice-saponin A3* | 9.67 | 983 > 351 | -185 | -58 |
| Ginsenoside Rf* | 9.71 | 845 > 799 | -150 | -33 |
| Uralsaponin U/Uralsaponin N | 9.90 | 837 > 351 | -185 | -58 |
| Isomer of uralsaponin C | 9.92 | 823 > 351 | -185 | -58 |
| 22*β*-acetoxyglycyrrhizin* | 9.93 | 879 > 351 | -185 | -58 |
| 24-Hydroxyl-licorice E2/Yunganoside M | 10.26 | 835 > 351 | -185 | -58 |
| 24-Hydroxy-licorice-saponin A3 | 10.38 | 999 > 351 | -185 | -58 |
| Macedonoside C | 10.56 | 821 > 351 | -185 | -58 |
| Ginsenoside Rg2* | 10.59 | 829 > 783 | -150 | -33 |
| Isomer of liquiritin | 10.60 | 417 > 255 | -101 | -30 |
| Ginsenoside Rh1* | 10.60 | 683 > 637 | -135 | -33 |
| d/e/f-*O*-Xyl(Ara)-GlcA-GlcA | 10.64 | 953 > 469 | -185 | -58 |
| 22-Hydroxy-licorice-saponin G2 | 10.67 | 853 > 501 | -185 | -58 |
| Ginsenoside Rb1* | 10.75 | 1153 > 1107 | -200 | -23 |
| 5,7-Dihydroxyl-flavone-4'-*O*-glucoside | 10.82 | 431 > 269 | -135 | -25 |
| Isomer of ginsenoside Rh1 | 10.82 | 683 > 637 | -135 | -33 |
| Vinaginsenoside R13 | 10.86 | 1025 > 979 | -200 | -33 |
| Acetyl-ginsenoside Re | 10.90 | 1033 > 987 | -200 | -33 |
| Licorice-saponin E2* | 10.98 | 819 > 351 | -185 | -58 |
| Licorice-saponin H2* | 10.99 | 821 > 351 | -185 | -58 |
| Uralsapionin D | 11.01 | 849 > 497 | -185 | -58 |
| Ginsenoside Rc* | 11.02 | 1123 > 1107 | -200 | -23 |
| Isomer of licorice-saponin H2 | 11.04 | 821 > 351 | -185 | -58 |
| Licorice-saponin G2* | 11.04 | 837 > 351 | -185 | -58 |
| Isoliquiritigenin* | 11.06 | 255 > 135 | -80 | -24 |
| Not identified | 11.08 | 851 > 351 | -185 | -58 |
| Ginsenoside Ro* | 11.09 | 955 > 793 | -200 | -50 |
| Isomer of 5'-hydroxy-4'-methoxyisoflavone-3'-*β*-D-glucoside | 11.21 | 461 > 299 | -125 | -25 |
| Isomer of licorice-saponin H2 | 11.24 | 821 > 351 | -185 | -58 |
| Isomer of calycosin-7-*O*-*β*-D-glucoside | 11.25 | 445 > 283 | -84 | -22 |

| | | | | |
|---|---|---|---|---|
| Ginsenoside Rb2* | 11.31 | 1123 > 1107 | -200 | -23 |
| Yunganoside E2 | 11.46 | 819 > 351 | -185 | -58 |
| 5-Hydroxy-liquiritin or 8-Hydroxy-liquiritin | 11.48 | 433 > 151 | -135 | -25 |
| Isomer of liquiritigenin-*O*-diglucoside | 11.50 | 579 > 255 | -135 | -25 |
| J/K/L-*O*-Xyl(Ara)-Rha-Glc | 11.50 | 961 > 915 | -150 | -33 |
| Formononetin* | 11.51 | 267 > 252 | -125 | -25 |
| Ginsenoside Rb3* | 11.52 | 1123 > 1077 | -200 | -23 |
| 24-Hydroxyl-licorice E2 | 11.56 | 835 > 483 | -185 | -58 |
| 5-Hydroxy-7-methoxyflavanone-5-*O*-glucoside | 11.60 | 447 > 285 | -125 | -25 |
| Acetyl-ginsenoside Re | 11.63 | 1033 > 987 | -200 | -33 |
| Ginsenoside Rg3* | 12.06 | 829 > 783 | -150 | -33 |
| Uralsaponin E | 12.17 | 835 > 483 | -185 | -58 |
| Ginsenoside Rd* | 12.25 | 991 > 945 | -200 | -33 |
| Isomucronulatol-*O*-apioside | 12.28 | 433 > 301 | -135 | -25 |
| Isomer of uralsaponin C | 12.38 | 823 > 351 | -185 | -58 |
| Genistin | 12.40 | 431 > 269 | -135 | -25 |
| Uralsaponin M | 12.51 | 879 > 351 | -185 | -58 |
| 22*β*-Acetoxyglycyrrhizic acid | 12.52 | 865 > 485 | -185 | -58 |
| Isomer of ginsenoside Rd | 12.54 | 991 > 945 | -200 | -33 |
| J/K/L-*O*-Glc-Rha-Xyl(Ara) | 12.56 | 961 > 915 | -150 | -33 |
| P-*O*-Glc-Glc-Glc-Glc | 12.72 | 1171 > 1125 | -200 | -33 |
| Isomer of calycosin-7-*O*-*β*-D-glucoside | 12.75 | 445 > 283 | -84 | -22 |
| G/H-*O*-Glc-Glc-Glc-Xyl(Ara)-Xyl(Ara) | 12.77 | 1255 > 1029 | -200 | -33 |
| Isomer of isoliquiritigenin-*O*-diglucoside | 13.00 | 579 > 255 | -135 | -25 |
| Isomer of ginsenoside Rg3 | 13.04 | 829 > 783 | -150 | -33 |
| Uralsaponin U/Uralsaponin N | 13.04 | 837 > 351 | -185 | -58 |
| Acetyl-ginsenoside Re | 13.09 | 1033 > 987 | -200 | -33 |
| Astragaloside II* | 13.10 | 871 > 825 | -150 | -36 |
| Isomucronulatol-7-*O*-*β*-D-glucoside | 13.30 | 463 > 301 | -125 | -25 |
| Re1/2/3,20-glu-Rf,Notoginsenoside N | 13.56 | 1007 > 961 | -200 | -33 |
| Acetyl-liquiritin/isoliquiritin | 13.63 | 459 > 255 | -135 | -25 |
| Yunganoside I2/Licorice saponin B2 | 13.64 | 807 > 351 | -185 | -55 |
| Uralsaponin U/Uralsaponin N | 13.73 | 837 > 351 | -185 | -58 |
| Isomer of ginsenoside Rd | 13.77 | 991 > 945 | -200 | -33 |
| Ginsenoside Ra1 | 13.78 | 1255 > 1209 | -200 | -50 |
| 22*β*-Acetoxy-licorice-saponin B2 | 13.95 | 865 > 527 | -185 | -58 |
| 22*β*-Acetoxyglycyrrhaldehyde | 13.96 | 863 > 351 | -185 | -58 |
| Isoastragaloside II* | 13.97 | 871 > 825 | -150 | -36 |
| M/N/O-*O*-Glc-Xyl(Ara) | 14.00 | 831 > 785 | -150 | -33 |
| Liquiritigenin/Isoliquiritigenin-*O*-diglucoside | 14.22 | 579 > 255 | -135 | -25 |
| Rhaoglycyrrhizin | 14.30 | 967 > 469 | -185 | -58 |
| 3,9-Dimethoxy-pterocarpane-10-*O*-glucoside-apioside | 14.47 | 593 > 299 | -125 | -35 |
| Pseudoginsenoside F11 | 14.57 | 845 > 799 | -150 | -33 |
| r-*O*-GlcA-Glc | 14.62 | 865 > 485 | -185 | -58 |

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|---|---|---|---|---|
| Isomer of ginsenoside Rg3 | 14.72 | 829 > 783 | -150 | -33 |
| Ginsenoside Rg6 | 14.79 | 811 > 765 | -150 | -33 |
| Quinquenoside R1 | 14.81 | 1195 > 1149 | -200 | -33 |
| Uralsaponin P | 14.90 | 823 > 351 | -185 | -58 |
| Astragaloside V | 15.02 | 991 > 945 | -200 | -33 |
| Glycyrrhizic acid* | 15.06 | 821 > 351 | -190 | -56 |
| Isomucronulatol-7-*O*-*β*-D-glucoside | 15.07 | 463 > 301 | -125 | -25 |
| 5-Hydroxy-liquiritin or 8-Hydroxy-liquiritin | 15.13 | 433 > 151 | -135 | -25 |
| Gypenoside XVII | 15.17 | 991 > 945 | -200 | -33 |
| Notoginsenoside R2 | 15.24 | 815 > 769 | -150 | -33 |
| Pseudoginsenoside Rc1 | 15.35 | 1033 > 987 | -200 | -33 |
| Ginsenoside F4* | 15.41 | 811 > 765 | -150 | -33 |
| Ginsenoside Rk1 | 15.55 | 811 > 765 | -150 | -33 |
| G/H-*O*-Glc-Glc-Xyl(Ara) | 15.75 | 961 > 915 | -150 | -33 |
| Glycyrflavoside C | 15.78 | 807 > 351 | -185 | -55 |
| Cyclogaleginoside D | 15.89 | 871 > 825 | -150 | -36 |
| Uralsaponin P | 16.03 | 823 > 351 | -185 | -58 |
| d/e/f-*O*-GlcA-Glc | 16.10 | 777 > 627 | -190 | -56 |
| Pseudoginsenoside Rc1 | 16.19 | 1033 > 987 | -200 | -33 |
| Notoginsenoside T5 | 16.25 | 797 > 751 | -150 | -33 |
| Astragaloside I | 16.32 | 913 > 867 | -150 | -32 |
| Isomer of ginsenoside Rg2 | 16.38 | 829 > 783 | -150 | -33 |
| 22*β*-Acetoxy-licorice-saponin B2 | 16.38 | 865 > 513 | -185 | -58 |
| Chikusetsusaponin Iva/Zingibroside R1 | 16.50 | 839 > 793 | -150 | -33 |
| Licorice saponin J2 | 16.63 | 823 > 351 | -185 | -58 |
| Notoginsenoside T5 | 16.75 | 797 > 751 | -150 | -33 |
| Astragaloside VI | 16.80 | 991 > 945 | -200 | -33 |
| Isoastragaloside I | 17.16 | 913 > 867 | -150 | -32 |
| Astragaloside IV* | 17.25 | 829 > 783 | -135 | -33 |
| Cyclosieversioside B | 17.29 | 913 > 867 | -150 | -32 |
| Ginsenoside Rh2 | 17.50 | 667 > 621 | -150 | -33 |
| Licorice-saponin B2 | 17.55 | 807 > 351 | -185 | -58 |
| Isomer of ginsenoside Rh2 | 17.82 | 667 > 621 | -150 | -33 |
| Resokaempferol | 17.87 | 269 > 133 | -125 | -25 |
| Ginsenoside Rs2 | 17.88 | 1165 > 1119 | -200 | -33 |
| Astragaloside III | 17.90 | 829 > 783 | -135 | -33 |
| Isomer of pratensein | 18.30 | 299 > 284 | -125 | -25 |
| Ginsenoside Rs2 | 18.37 | 1165 > 1119 | -200 | -33 |
| Acetyl-Liquiritin/Isoliquiritin | 18.56 | 459 > 255 | -135 | -25 |
| Quinquenoside R1 | 18.74 | 1195 > 1149 | -200 | -33 |
| 3-Hydroxy-9,10-dimethoxy-pterocarpane | 18.90 | 299 > 284 | -125 | -25 |
| 10-Hydroxy-3,9-dimethoxy-pterocarpane | 19.01 | 299 > 284 | -125 | -25 |
| Ginsenoside Rs2 | 19.25 | 1165 > 1119 | -200 | -33 |
| Pseudoginsenoside Rc1 | 19.53 | 1033 > 987 | -200 | -33 |

| | | | | |
|---|---|---|---|---|
| Pseudoginsenoside Rc1 | 19.73 | 1033 > 987 | -200 | -33 |
| Ginsenoside Rs2 | 19.79 | 1165 > 1119 | -200 | -33 |
| Ginsenoside Rs4/Rs5 | 20.00 | 853 > 807 | -150 | -33 |
| Ginsenoside Rg5* | 20.13 | 811 > 765 | -150 | -33 |
| Ginsenoside Rs4/Rs5 | 21.57 | 853 > 807 | -150 | -33 |

*: the compound quantitated with the reference.

**Table S3 The linear regression data, limits of quantification (LOQs) and detection (LODs) for all targeted 36 analytes.**

| Analytes | $t_R$(min) | Regression equation | $r^2$ | Linear range (μg/mL) | LOD (ng/mL) | LOQ (ng/mL) |
|---|---|---|---|---|---|---|
| Apigenin-6,8-di-*C*-*β*-D-glucopyranoside (**1**) | 3.43 | y=0.0001x+0.0244 | 0.9997 | 0.2-28.06 | 7.23 | 22.20 |
| Calycosin-7-*O*-*β*-D-glucoside (**2**) | 4.64 | y=0.00002x+0.00035 | 0.9999 | 0.2-24.05 | 6.78 | 18.89 |
| Liquiritin (**3**) | 4.67 | y=0.0002x+0.013 | 0.9997 | 0.03-14.6 | 0.87 | 2.80 |
| Liquiritin aposide (**4**) | 4.77 | y=0.00001x+0.00042 | 0.9996 | 0.05-12.30 | 4.12 | 12.01 |
| Isoliquiritin aposide (**5**) | 7.06 | y=0.00001x-0.00075 | 0.9998 | 0.2-12.07 | 5.78 | 25.00 |
| Ginsenoside Rg1 (**6**) | 7.10 | y=0.0005x+0.0481 | 0.9991 | 0.02-13.00 | 4.12 | 12.01 |
| Ginsenoside Re (**7**) | 7.15 | y=0.00001x+0.000673 | 0.9991 | 0.01-4.50 | 3.50 | 17.66 |
| Isoliquiritin (**8**) | 7.17 | y=0.0005x+0.0125 | 0.9997 | 0.01-5.33 | 0.04 | 0.20 |
| Liquiritigenin (**9**) | 7.26 | y=0.001x+0.0618 | 0.9991 | 0.1-12.00 | 0.31 | 0.75 |
| Ononin (**10**) | 7.28 | y=0.0003x-0.0213 | 0.9995 | 0.03-6.88 | 0.45 | 1.34 |
| Calycosin (**11**) | 8.11 | y=0.0025x+0.2172 | 0.9997 | 0.02-8.77 | 0.09 | 0.17 |
| Uralsaponin C (**12**) | 8.19 | y=0.000047x-0.059422 | 0.9993 | 0.1-4.17 | 7.51 | 13.01 |
| Uralsaponin F (**13**) | 8.88 | y=0.0007x-0.0826 | 0.9996 | 0.15-5.04 | 3.95 | 15.75 |
| Licorice saponin A3 (**14**) | 9.67 | y=0.00004x-0.03274 | 0.999 | 0.78-25.14 | 4.09 | 9.80 |
| Ginsenoside Rf (**15**) | 9.71 | y=0.0017x+0.0140 | 0.9993 | 0.01-3.26 | 0.87 | 3.18 |
| 22*β*-Acetoxyglycyrrhizin (**16**) | 9.93 | y=0.0006x-0.3618 | 0.9996 | 0.70-23.76 | 23.21 | 46.41 |
| Ginsenoside Rg2 (**17**) | 10.59 | y=0.0008x+0.4031 | 0.9994 | 0.1-9.40 | 4.52 | 9.20 |
| Ginsenoside Rh1 (**18**) | 10.60 | y=0.00005x+0.01752 | 0.9997 | 0.1-13.12 | 2.10 | 5.27 |
| Ginsenoside Rb1 (**19**) | 10.75 | y=0.0001x+0.0076 | 0.999 | 0.02-8.0 | 4.21 | 15.73 |
| Licorice saponin E2 (**20**) | 10.98 | y=0.0001x-0.2117 | 0.9995 | 0.13-16.63 | 4.78 | 30.12 |
| Licorice saponin H2 (**21**) | 10.99 | y=0.0011x-0.0176 | 0.999 | 0.02-1.3 | 0.74 | 1.48 |
| Ginsenoside Rc (**22**) | 11.02 | y=0.00003x+0.00566 | 0.9991 | 0.1-14.0 | 13.59 | 27.18 |
| Licorice saponin G2 (**23**) | 11.04 | y=0.0006x-0.3835 | 0.9995 | 0.1-13.22 | 7.56 | 25.08 |
| Isoliquiritigenin (**24**) | 11.06 | y=0.0003x-0.1192 | 0.999 | 0.02-4.45 | 3.21 | 8.64 |
| Ginsenoside Ro (**25**) | 11.09 | y=0.00001x+0.0032 | 0.9993 | 0.14-19.0 | 10.34 | 37.18 |
| Ginsenoside Rb2 (**26**) | 11.31 | y=0.0001x+0.0005 | 0.9994 | 0.05-7.07 | 6.90 | 55.25 |
| Fermononetin (**27**) | 11.34 | y=0.0019x-0.0286 | 0.9998 | 0.01-3.35 | 0.21 | 0.65 |
| Ginsenoside Rb3 (**28**) | 11.52 | y=0.0001x+0.0057 | 0.9999 | 0.10-10.75 | 3.80 | 8.10 |
| Ginsenoside Rg3 (**29**) | 12.06 | y=0.0006x+0.0853 | 0.9993 | 0.06-16.57 | 8.82 | 32.25 |
| Ginsenoside Rd (**30**) | 12.25 | y=0.0003x+0.0014 | 0.9996 | 0.20-2.34 | 2.28 | 4.56 |
| Astragaloside II (**31**) | 13.10 | y=0.0001x+0.0032 | 0.9997 | 0.03-8.24 | 8.05 | 32.21 |
| Isoastragaloside II (**32**) | 13.97 | y=0.00001x+0.00129 | 0.9992 | 0.05-6.39 | 5.65 | 24.96 |
| Glycyrrhizinic acid (**33**) | 15.06 | y=0.0007x-1.469 | 0.999 | 0.077-4.96 | 2.68 | 9.68 |
| Ginsenoside F4 (**34**) | 15.41 | y=0.0001x-0.016 | 0.9995 | 0.05-13.01 | 2.14 | 9.06 |
| Astragaloside IV (**35**) | 17.25 | y=0.0005x+0.0052 | 0.9998 | 0.02-2.21 | 2.15 | 8.61 |
| Ginsenoside Rg5 (**36**) | 20.13 | y=0.0004x+0.013 | 0.9996 | 0.01-7.55 | 1.21 | 4.75 |

**Table S4 The inter-day, intra-day precision, recovery performance, repeatability, and stability validation data for all monitored analytes ($n$ = 6).**

| Analytes | Intra-day RSD (%) | Inter-day RSD (%)[a] | Recovery (%) | RSD (%) | Repeatability RSD (%) | Stability RSD (%) |
|---|---|---|---|---|---|---|
| Apigenin-6,8-di-*C*-*β*-D-glucopyranoside (**1**) | 3.73 | 4.20 | 100.82 | 10.29 | 4.40 | 3.29 |
| Calycosin-7-*O*-*β*-D-glucoside (**2**) | 4.07 | 4.96 | 106.86 | 8.51 | 2.99 | 4.22 |
| Liquiritin (**3**) | 4.16 | 4.62 | 100.84 | 8.54 | 4.78 | 4.02 |
| Liquiritin aposide (**4**) | 2.66 | 3.88 | 100.72 | 7.46 | 4.10 | 4.76 |
| Isoliquiritin aposide (**5**) | 4.61 | 4.99 | 102.04 | 3.11 | 3.14 | 1.11 |
| Ginsenoside Rg1 (**6**) | 4.45 | 4.83 | 102.86 | 7.31 | 4.45 | 3.02 |
| Ginsenoside Re (**7**) | 2.98 | 4.30 | 101.27 | 7.26 | 2.83 | 4.11 |
| Isoliquiritin (**8**) | 3.76 | 3.95 | 101.29 | 11.06 | 2.70 | 4.16 |
| Liquiritigenin (**9**) | 1.70 | 3.45 | 103.49 | 5.01 | 2.55 | 2.55 |
| Ononin (**10**) | 3.16 | 4.61 | 99.91 | 6.28 | 4.10 | 4.06 |
| Calycosin (**11**) | 2.96 | 3.65 | 96.13 | 6.39 | 3.08 | 1.71 |
| Uralsaponin C (**12**) | 2.82 | 3.69 | 106.72 | 4.35 | 5.01 | 4.72 |
| Uralsaponin F (**13**) | 3.75 | 5.25 | 101.15 | 9.95 | 1.43 | 3.44 |
| Licorice saponin A3 (**14**) | 2.55 | 3.76 | 100.88 | 7.70 | 1.41 | 4.29 |
| Ginsenoside Rf (**15**) | 1.95 | 4.13 | 99.89 | 11.28 | 1.32 | 1.19 |
| 22*β*-Acetoxyglycyrrhizin (**16**) | 1.64 | 3.07 | 99.59 | 9.84 | 2.04 | 3.01 |
| Ginsenoside Rg2 (**17**) | 3.57 | 4.57 | 98.58 | 12.65 | 4.98 | 3.71 |
| Ginsenoside Rh1 (**18**) | 3.44 | 3.49 | 90.68 | 6.27 | 2.16 | 2.92 |
| Ginsenoside Rb1 (**19**) | 3.54 | 4.72 | 102.72 | 4.86 | 2.92 | 1.71 |
| Licorice saponin E2 (**20**) | 0.96 | 2.37 | 108.92 | 4.67 | 4.23 | 4.23 |
| Licorice saponin H2 (**21**) | 3.89 | 3.68 | 103.82 | 8.32 | 3.52 | 3.47 |
| Ginsenoside Rc (**22**) | 1.97 | 3.72 | 108.15 | 12.07 | 2.68 | 2.96 |
| Licorice saponin G2 (**23**) | 3.11 | 3.33 | 107.20 | 9.95 | 3.55 | 4.03 |
| Isoliquiritigenin (**24**) | 3.13 | 3.25 | 106.87 | 4.41 | 3.27 | 4.44 |
| Ginsenoside Ro (**25**) | 2.72 | 4.14 | 103.77 | 11.20 | 2.40 | 4.41 |
| Ginsenoside Rb2 (**26**) | 3.41 | 4.93 | 103.68 | 3.74 | 4.26 | 4.63 |
| Fermononetin (**27**) | 1.48 | 1.39 | 100.37 | 5.30 | 3.15 | 4.77 |
| Ginsenoside Rb3 (**28**) | 4.56 | 4.73 | 109.91 | 10.01 | 3.93 | 3.93 |
| Ginsenoside Rg3 (**29**) | 2.86 | 3.58 | 103.21 | 13.21 | 4.42 | 4.42 |
| Ginsenoside Rd (**30**) | 3.48 | 3.97 | 99.50 | 8.97 | 4.04 | 4.94 |
| Astragaloside II (**31**) | 2.81 | 2.53 | 97.97 | 13.81 | 3.73 | 3.76 |
| Isoastragaloside II (**32**) | 2.65 | 4.60 | 98.78 | 12.31 | 3.81 | 3.81 |
| Glycyrrhizinic acid (**33**) | 3.12 | 2.88 | 97.08 | 10.86 | 1.85 | 3.14 |
| Ginsenoside F4 (**34**) | 2.85 | 3.50 | 102.31 | 9.78 | 4.67 | 4.67 |
| Astragaloside IV (**35**) | 2.74 | 4.70 | 97.01 | 7.79 | 2.78 | 3.86 |
| Ginsenoside Rg5 (**36**) | 3.25 | 4.07 | 107.21 | 3.67 | 4.54 | 4.24 |

[a]: $n$ = 3