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**Supporting Information**

# Integration of a hybrid scan approach and in-house high-resolution $MS^2$ spectral database for characterizing the multicomponents of Xuebijing Injection

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# Content

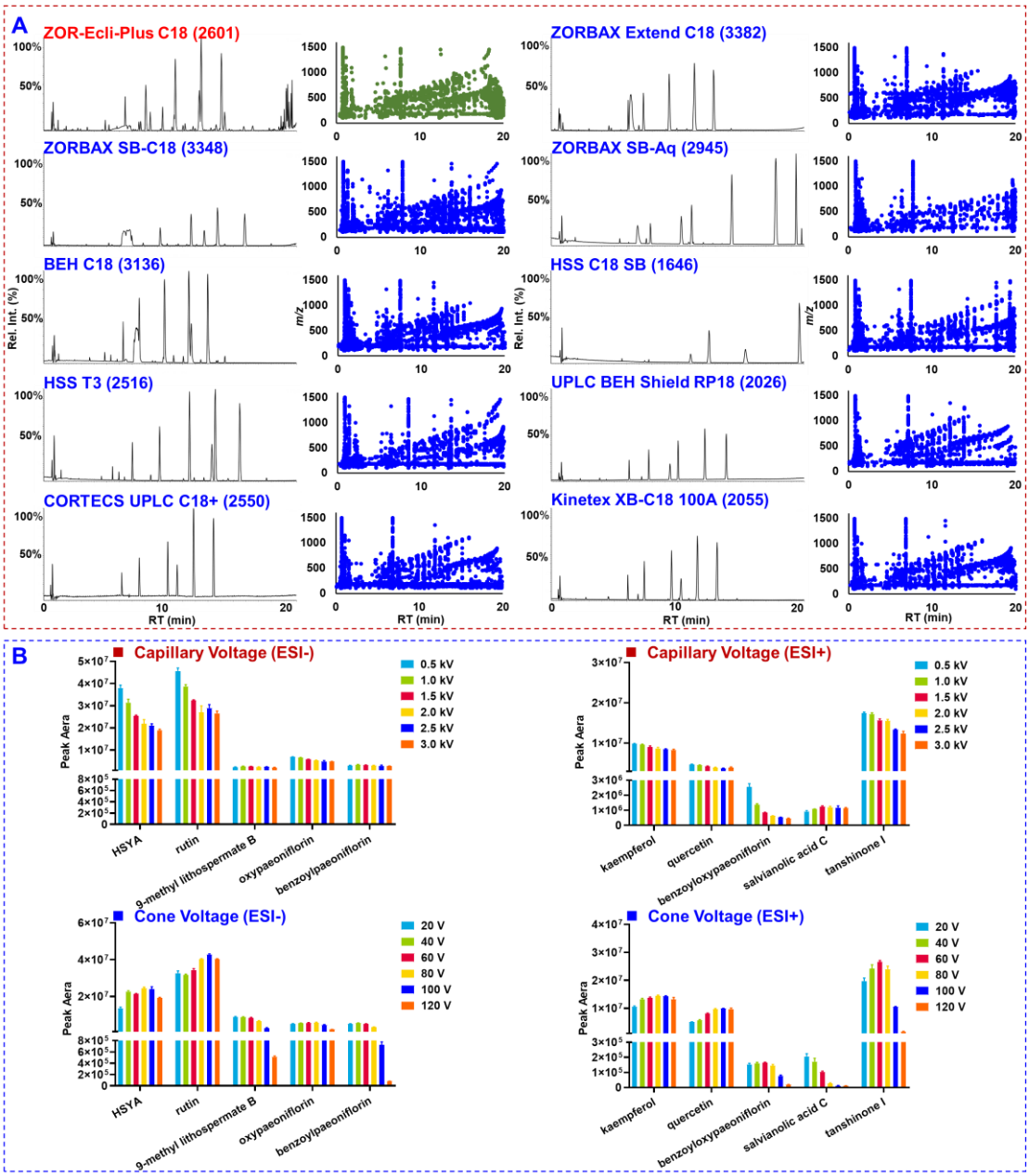


**Fig. S1** Method development of UHPLC/IM-QTOF-MS for characterizing the multicomponents from XBJ Injection. **A**-Stationary phase screening (the left shows the base peak intensity-BPI chromatograms obtained on 10 candidate columns; the right is the scatter plot of the peaks resolved by both MS and chromatographic separation on each column); **B**-optimization of capillary voltage and cone voltage in both the positive and negative ESI modes for the Vion IM-QTOF mass spectrometer ($n$=3).

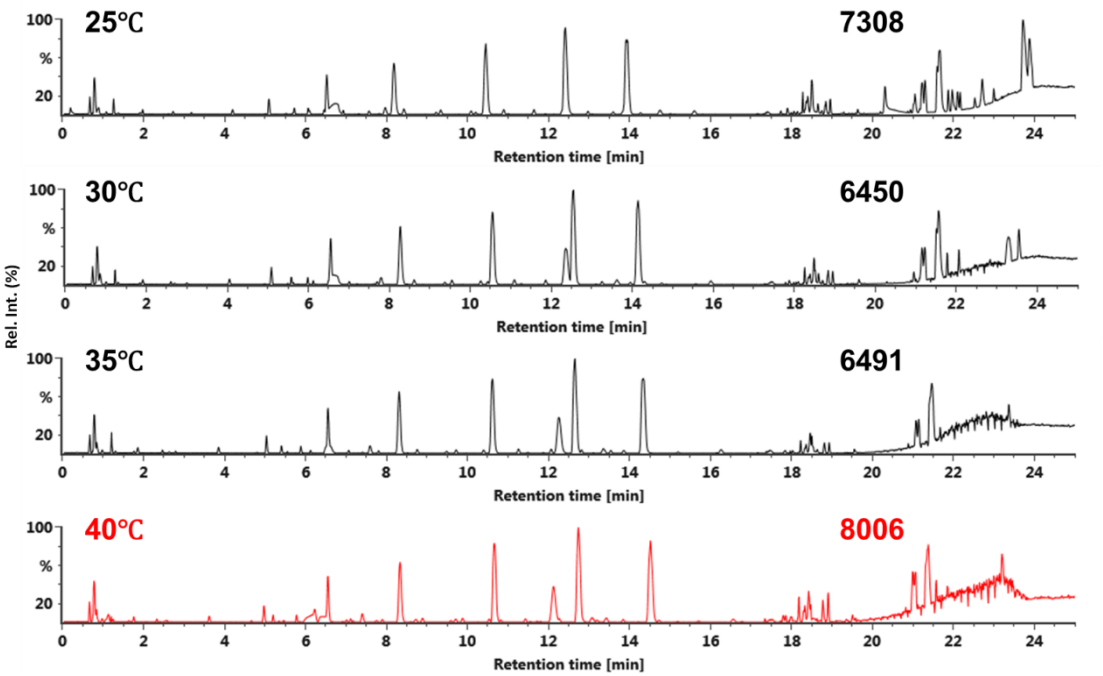


**Fig. S2** Method development by optimizing the column temperature on the selected Zorbax Eclipse Plus C18 column, showing the base peak intensity chromatogram and the number of peaks resolved from XBJ Injection.

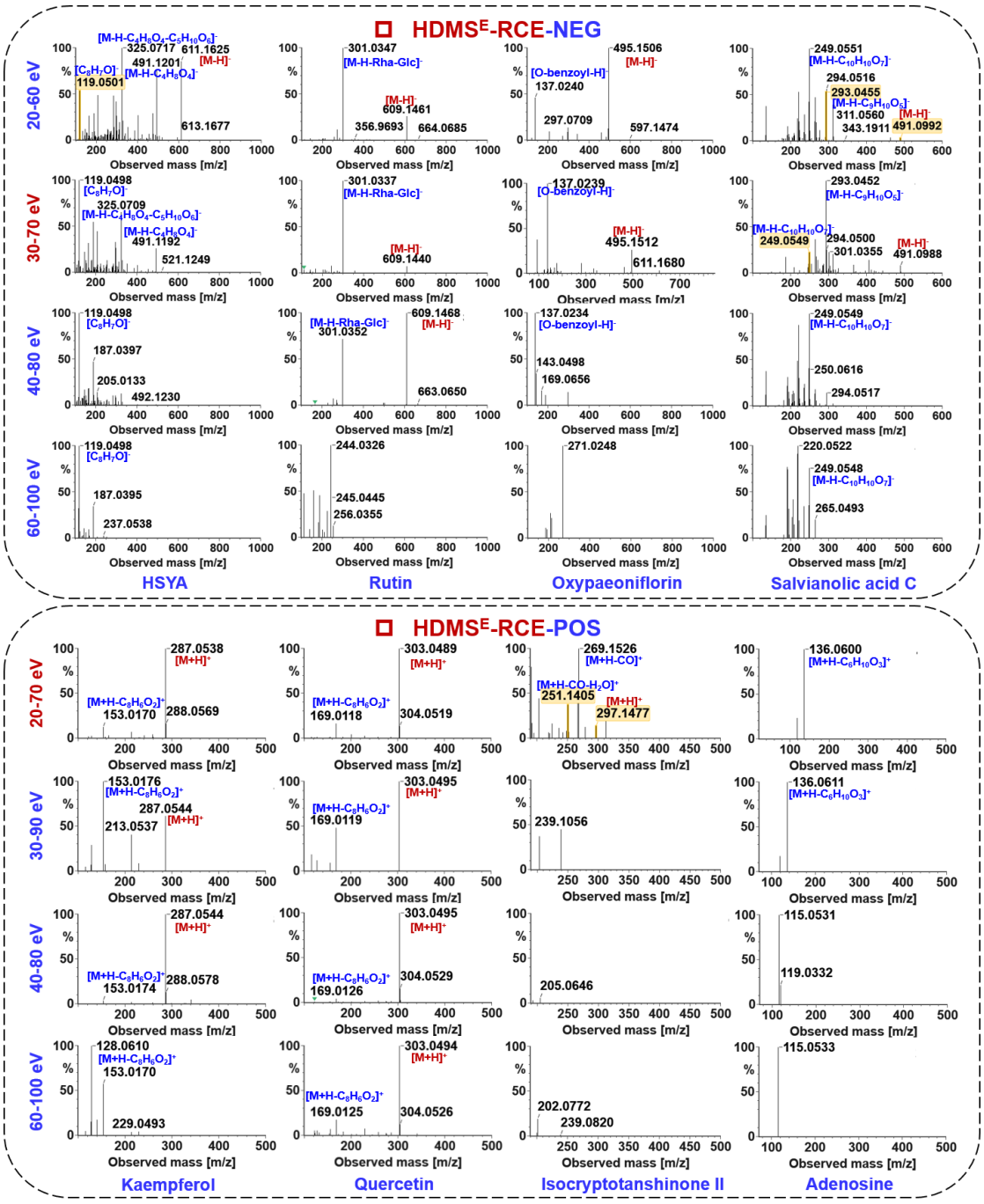


**Fig. S3** Method development by optimizing ramp collision energy (RCE) for the HDMS$^E$ approach established both in the negative and positive ESI modes, using the representative compounds of XBJ Injection as the case.

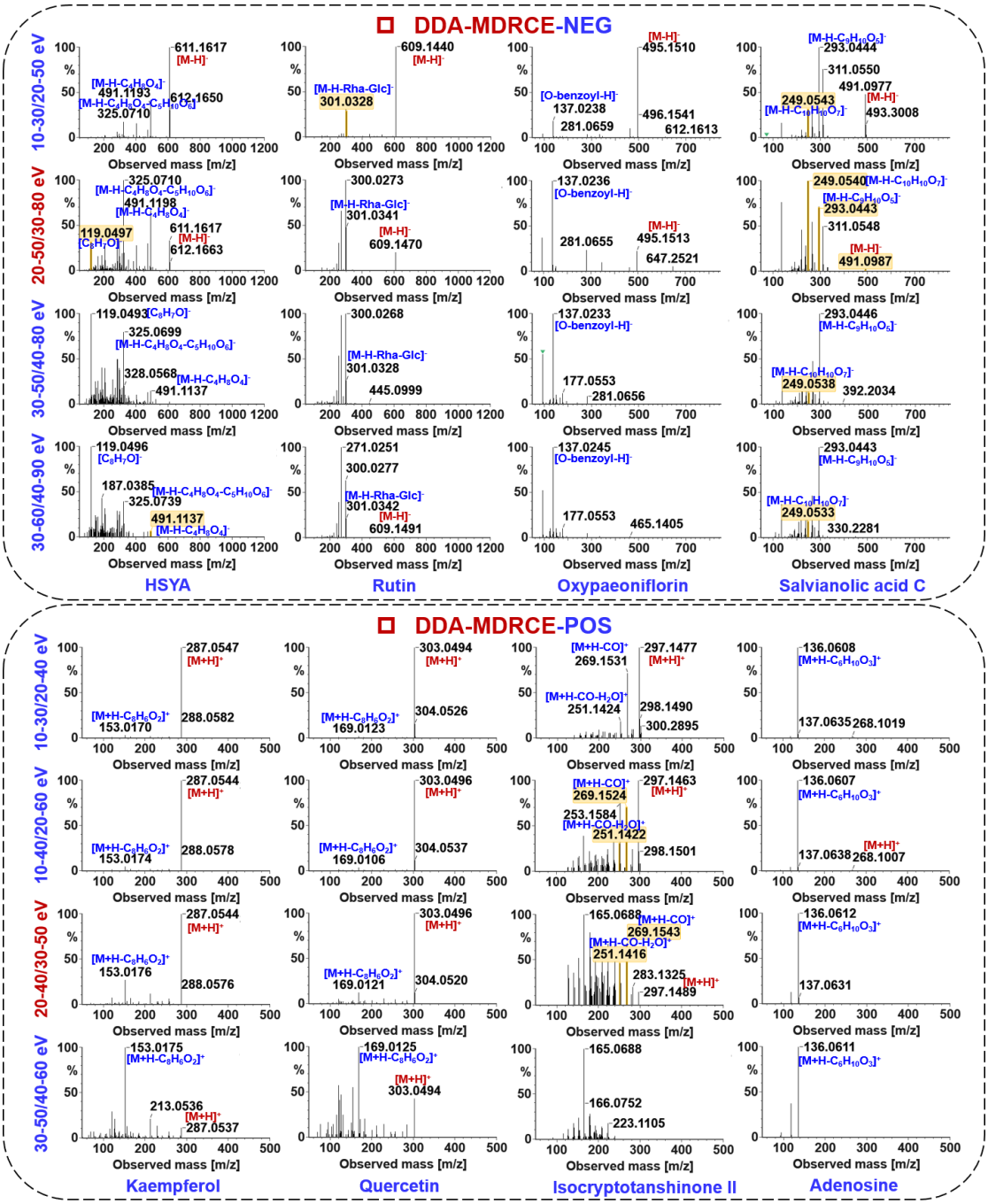


**Fig. S4** Method development by optimizing mass-dependent ramp collision energy (MDRCE) for the DDA approach established both in the negative and positive ESI modes, using the representative compounds of XBJ Injection as the case.

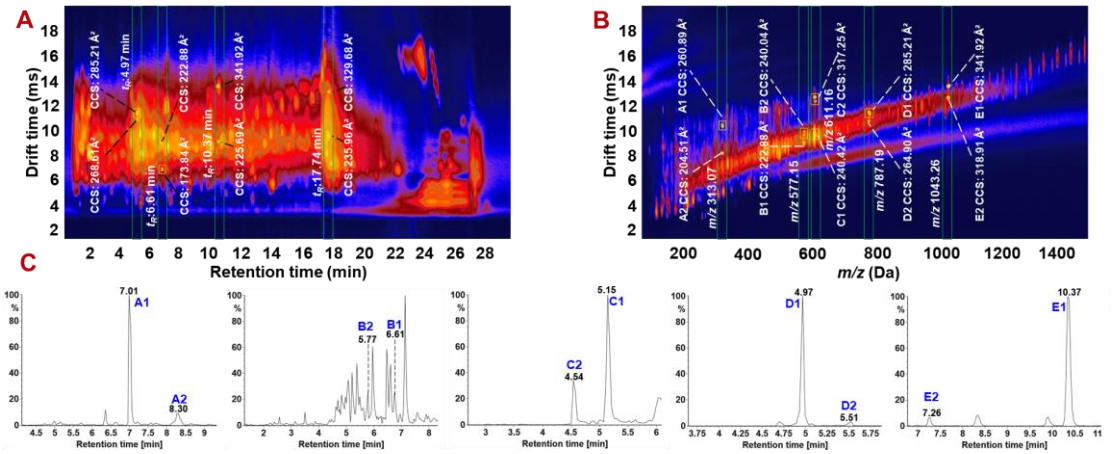


**Fig. S5** Two-dimensional heat map view of the ion mobility data showing the separation of co-eluting components (**A**: drift time VS $t_R$), the separation of isomers (**B**: drift time VS *m/z*), and the negative extraction ion chromatograms (EIC) of isomer compounds (**C**).

**Table S1** Information of 56 reference compounds used in this work.

| No. | Compound | Formula | M.W. | RT (min) | Type |
|---|---|---|---|---|---|
| **1** | Gallic acid | $C_7H_6O_5$ | 170.0215 | 12.00 | Organic acid |
| **2** | Methyl gallate | $C_8H_8O_5$ | 184.0372 | 5.40 | |
| **3** | Ethyl gallate | $C_9H_{10}O_5$ | 198.0528 | 7.42 | |
| **4** | Vanillic acid | $C_8H_8O_4$ | 168.0423 | 4.53 | |
| **5** | Vanillin | $C_8H_8O_3$ | 152.0473 | 7.18 | |
| **6** | Ferulic acid | $C_{10}H_{10}O_4$ | 194.0579 | 8.39 | |
| **7** | Ethyl ferulate | $C_{12}H_{14}O_4$ | 222.0892 | 18.18 | |
| **8** | Danshensu | $C_9H_{10}O_5$ | 198.0528 | 12.62 | |
| **9** | *p*-Coumaric acid | $C_9H_8O_3$ | 164.0473 | 18.11 | |
| **10** | Caffeic acid | $C_9H_8O_4$ | 180.0423 | 5.73 | |
| **11** | Salvianolic acid B | $C_{36}H_{30}O_{16}$ | 718.1534 | 15.34 | |
| **12** | 9-Methyl lithospermate B | $C_{37}H_{32}O_{16}$ | 732.1690 | 17.47 | |
| **13** | Dimethyl lithospermate B | $C_{38}H_{34}O_{16}$ | 746.1847 | 17.87 | |
| **14** | Chlorogenic acid | $C_{16}H_{18}O_9$ | 354.0951 | 5.35 | |
| **15** | Protocatechuate | $C_7H_6O_4$ | 154.0266 | 9.80 | |
| **16** | Protocatechuic aldehyde | $C_7H_6O_3$ | 138.0317 | 8.39 | |
| **17** | Lithospermic acid | $C_{27}H_{22}O_{12}$ | 538.1111 | 15.33 | |
| **18** | Salvianolic acid C | $C_{26}H_{20}O_{10}$ | 492.1056 | 17.58 | |
| **19** | Salvianolic acid A | $C_{26}H_{22}O_{10}$ | 494.1213 | 13.38 | |
| **20** | Salvianolic acid F | $C_{17}H_{14}O_6$ | 314.0790 | 11.90 | |
| **21** | Rosmarinic acid | $C_{18}H_{16}O_8$ | 360.0845 | 12.58 | |
| **22** | Tanshinone I | $C_{18}H_{12}O_3$ | 276.0786 | 20.93 | Phenanthrenequinone |
| **23** | Tanshinone IIA | $C_{19}H_{18}O_3$ | 294.1256 | 22.38 | |
| **24** | Dihydrotanshinone I | $C_{18}H_{14}O_3$ | 278.0943 | 19.89 | |
| **25** | Cryptotanshinone | $C_{19}H_{20}O_3$ | 296.1412 | 21.03 | |
| **26** | Catechin | $C_{15}H_{14}O_6$ | 290.079 | 5.33 | Flavonoid |
| **27** | Apigenin | $C_{15}H_{10}O_5$ | 270.0528 | 17.78 | |
| **28** | Myricetin | $C_{15}H_{10}O_8$ | 318.0376 | 12.36 | |
| **29** | Luteolin | $C_{15}H_{10}O_6$ | 286.0477 | 17.85 | |
| **30** | Quercetin | $C_{15}H_{10}O_7$ | 302.0427 | 17.33 | |
| **31** | Kaempferol | $C_{15}H_{10}O_6$ | 286.0477 | 17.83 | |
| **32** | Kaempferol-7-*O*-glucoside | $C_{21}H_{20}O_{11}$ | 448.1006 | 11.29 | |
| **33** | Kaempferol-3-*O*-glucoside | $C_{21}H_{20}O_{11}$ | 448.1006 | 9.63 | |
| **34** | Kaempferol-3-*O*-rutinoside | $C_{27}H_{30}O_{15}$ | 594.1585 | 10.66 | |
| **35** | Quercetin-7-*O*-*β*-D-glucoside | $C_{21}H_{20}O_{12}$ | 464.0955 | 9.20 | |
| **36** | Rutin | $C_{27}H_{30}O_{16}$ | 610.1534 | 8.56 | |
| **37** | Isoquercitrin | $C_{21}H_{20}O_{12}$ | 464.0955 | 8.38 | |

| | | | | | |
|---|---|---|---|---|---|
| **38** | Quercetin-3-*O*-*β*-D-glucose-7-*O*-*β*-D-gentiobioside | $C_{33}H_{40}O_{22}$ | 788.2011 | 4.98 | |
| **39** | Luteoloside | $C_{21}H_{20}O_{11}$ | 448.1006 | 9.48 | |
| **40** | Isorhamnetin-3-*O*-glucoside | $C_{22}H_{22}O_{12}$ | 478.1110 | 11.87 | |
| **41** | Isorhamnetin-7-*O*-glucoside | $C_{22}H_{22}O_{12}$ | 478.1110 | 11.44 | |
| **42** | Hyperoside | $C_{21}H_{20}O_{12}$ | 464.0955 | 9.17 | |
| **43** | 5,7,4'-Trihydroxy-6-methoxyflavone-3-*O*-*β*-D-rutinoside | $C_{28}H_{32}O_{16}$ | 624.1690 | 11.27 | |
| **44** | (2*S*)-4',5,6,7-Tetrahydroxy-flavanone 6-*O*-*β*-D-glucoside | $C_{21}H_{22}O_{11}$ | 450.1162 | 9.84 | |
| **45** | Hydroxysafflor yellow A | $C_{27}H_{32}O_{16}$ | 612.1690 | 5.15 | |
| **46** | Anhydrosafflor yellow B | $C_{48}H_{52}O_{26}$ | 1044.2747 | 10.35 | |
| **47** | Oxypaeoniflorin | $C_{23}H_{28}O_{12}$ | 496.1581 | 5.23 | |
| **48** | Benzoylpaeoniflorin | $C_{30}H_{32}O_{12}$ | 584.1894 | 17.74 | Terpenoid |
| **49** | Benzoyloxypaeoniflorin | $C_{30}H_{32}O_{13}$ | 600.1843 | 15.73 | |
| **50** | 5-Hydroxymethylfurfural | $C_6H_6O_3$ | 126.0317 | 2.71 | |
| **51** | Levistilide A | $C_{24}H_{28}O_4$ | 380.1988 | 22.13 | |
| **52** | Senkyunolide I | $C_{12}H_{16}O_4$ | 224.1049 | 12.93 | Phthalide |
| **53** | *N*-butylidenephthalide | $C_{12}H_{12}O_2$ | 188.0837 | 14.09 | |
| **54** | Ligustilide | $C_{12}H_{14}O_2$ | 190.0994 | 22.16 | |
| **55** | Uridine | $C_9H_{12}N_2O_6$ | 244.0695 | 0.72 | Nucleoside |
| **56** | Adenosine | $C_{10}H_{13}N_5O_4$ | 267.0968 | 2.66 | |

**Table S2** Detailed information of ten candidate columns tested in the stationary phase screening for method development.

| No. | Chromatographic column | Specification/Manufacturer | Separation characteristics |
|---|---|---|---|
| 1 | ZORBAX Eclipse Plus C18 | 2.1×100 mm, 1.8 μm; Agilent | Filled with high-performance particulate C18 filler, this column could be used for the analysis of acidic and neutral samples, especially for the separation of alkaline compounds with poor peak shape on other chromatographic columns. |
| 2 | ZORBAX SB-C18 | 2.1×100 mm, 1.8 μm; Agilent | This SB-C18 column has diisobutyl side-chain radical and can provide the best stability under the condition of low pH mobile phase. |
| 3 | BEH C18 | 2.1×100 mm, 1.7 μm; Waters | Built on the BEH particle platform, this column has the widest usable pH range (pH 1–12), which is ideal for the separation of medium or weak polar compounds. |
| 4 | HSS T3 | 2.1×100 mm, 1.8 μm; Waters | The universal, silica-based bonded phase used for the HSS T3 sorbents is compatible with 100% aqueous mobile phase and can enhance retention of polar molecules. |
| 5 | CORTECS UPLC C18+ | 2.1×100 mm, 1.6 μm; Waters | CORTECS C18 columns are general purpose, high-efficiency columns based on a solid-core particle that offer balanced retention of acids, bases and neutrals at low and mid-range pH. |
| 6 | ZORBAX Extend C18 | 2.1×100 mm, 1.8 μm; Agilent | The column incorporates a unique patented bidentate silane, combined with a double-endcapping process that protects the silica from dissolution at high pH, which also has good separations of peptides, polypeptides, and small proteins from pH 2–11.5. |
| 7 | HSS C18 SB | 2.1×100 mm, 1.8 μm; Waters | HSS C18 SB column has the unique non-end-capped, low-coverage silica-based C18 chemistry, which is used for low pH separations that contain complex mixtures of basic and |

| | | | |
|---|---|---|---|
| | | | non-basic compounds. |
| 8 | ZORBAX SB-Aq | 2.1×100 mm, 1.8 μm; Agilent | This SB-Aq column has diisopropyl side-chain radical and is compatible with 100% pure water mobile phase, which can be used for high acid mobile phase. |
| 9 | BEH Shield RP18 | 2.1×100 mm, 1.7 μm; Waters | The embedded carbamate group in the bonded phase ligand provides alternate selectivity, especially for phenolic compounds compared to straight chain alkyl columns. This allows for alternate selectivity to that of alkyl reversed-phase columns and aqueous mobile phase compatibility. |
| 10 | Kinetex XB-C18 | 2.1×100 mm, 1.7 μm; Phenomenex | As a phenyl shell core column, it is stable in 100% aqueous solution and can provide excellent reverse hydrophobic retention and polar selectivity to aromatic compounds. |

**Table S3** Detailed information of the 294 components characterized from the XBJ Injection.

| No. | Observed *m/z* | Mass error (ppm) | Observed RT (min) | Expected CCS (Å²) | Observed CCS (Å²) | CCS delta (%) | Formula | Adducts | Identification | Original | Type | $MS^2$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 353.0837 | –1.7 | 0.85 | | 166.99 | | $C_{14}H_{18}O_9$ | $[M+Na]^+$ | woodorien or its isomer | SMRR | OT | 337.1089, 298.1135, 203.0516, 122.0583 |
| 2 | 665.2148 | 0.3 | 0.86 | 235.29 | 233.26 | –0.86 | $C_{24}H_{42}O_{21}$ | $[M–H]^–$ | stachyose or its isomer | SMRR | OT | 503.1612, 383.1188, 341.1083, 209.0660, 191.0553 |
| 3 | 683.2255 | 9.0 | 0.88 | 230.72 | 231.12 | 0.17 | $C_{31}H_{40}O_{17}$ | $[M–H]^–$ | chuanxiongoside B or its isomer | CR | PP | 665.2149, 503.1612, 383.1188, 341.1083, 113.0239 |
| 4 | 179.0553 | –4.8 | 0.88 | 231.97 | 232.61 | 0.27 | $C_6H_{12}O_6$ | $[M–H]^–$ | fructose or its isomer | SMRR | OT | 161.0444, 143.0343, 119.0339, 59.0136 |
| 5 | 377.0854 | –6.3 | 0.88 | 169.00 | 170.46 | 0.86 | $C_{18}H_{18}O_9$ | $[M–H]^–$ | isomer of salvianolic acid C | SMRR | OA | 341.1084, 179.0553, 143.0338 |
| 6 | 503.1615 | –0.4 | 0.92 | 203.49 | 203.59 | 0.05 | $C_{18}H_{32}O_{16}$ | $[M–H]^–$ | raffitrinose or its isomer | SMRR | OT | 438.0461, 207.0503, 179.0554, 78.9584 |
| 7 | 268.1026 | –5.3 | 0.98 | 155.07 | 155.30 | 0.15 | $C_{10}H_{13}N_5O_4$ | $[M+H]^+$ | isomer of adenosine | CF | OT | 242.1013, 214.1062, 136.0601, 80.0471 |
| 8 | 119.0333 | –5.1 | 1.08 | 121.70 | 122.35 | 0.53 | $C_4H_6O_4$ | $[M+H]^+$ | isomer of succinic acid | SMRR | OA | 119.0331 |
| 9 | 134.0465 | –5.5 | 1.13 | 115.78 | 116.69 | 0.79 | $C_5H_5N_5$ | $[M–H]^–$ | isomer of adenine | CF | OT | 134.0465, 107.0358 |
| 10 | 593.1504 | –1.3 | 1.29 | | 234.83 | | $C_{27}H_{30}O_{15}$ | $[M–H]^–$ | kaempferol-3-*O*-*α*-l-rhamnopyranosyl-(1→6)-*β*-D-glucopyranoside or its isomer | SMRR | FL | 473.1078, 341.0656, 267.0644, 89.0236 |
| 11 | 274.0910 | –0.2 | 1.59 | | 152.99 | | $C_{10}H_{13}N_5O_3$ | $[M+Na]^+$ | 2'-deoxyadenosine or its isomer | ASR | OT | 221.0000, 193.0052, 155.9728, 137.9616, 110.9515 |
| 12 | 747.1908 | –3.0 | 1.64 | | 241.26 | | $C_{38}H_{36}O_{16}$ | $[M–H]^–$ | dimethyl salvianolic acid B or its isomer | SMRR | OA | 649.2186, 517.1763, 191.0553 |
| 13 | 375.1289 | –2.1 | 2.02 | 258.96 | 256.09 | –1.11 | $C_{16}H_{24}O_{10}$ | $[M–H]^–$ | isomer of desbenzoylpaeoniflorin | PRR | TP | 345.1179, 327.1075, 165.0548, 123.0442 |
| 14 | 252.1077 | –5.8 | 2.02 | | 152.48 | | $C_{10}H_{13}N_5O_3$ | $[M+H]^+$ | 2'-deoxyadenosine or its isomer | ASR | OT | 136.0732, 110.0629 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 15 | 195.0655 | –3.8 | 2.38 | 189.14 | 189.33 | 0.10 | $C_{10}H_{12}O_4$ | $[M+H]^+$ | paeonilactone B or its isomer | PRR | TP | 195.0655, 183.0656, 151.0751, 121.0649 |
| 16 | 213.0763 | –2.6 | 2.38 | 189.04 | 189.35 | 0.16 | $C_{10}H_{14}O_5$ | $[M–H]^–$ | isopaeonisuffial or its isomer | PRR | TP | 213.0763, 195.0655, 183.0656, 139.0760 |
| 17 | 331.0667 | –1.1 | 2.50 | 170.76 | 170.44 | –0.19 | $C_{13}H_{16}O_{10}$ | $[M–H]^–$ | 1-*O*-galloylglucose or its isomer | PRR | OT | 331.0668, 214.0658, 151.0032 |
| 18 | 119.0331 | –6.5 | 2.66 | 122.21 | 121.05 | –0.95 | $C_4H_6O_4$ | $[M+H]^+$ | isomer of succinic acid | ASR | OA | 92.0216 |
| 19* | 268.1024 | –5.9 | 2.66 | 152.65 | 152.07 | –0.38 | $C_{10}H_{13}N_5O_4$ | $[M+H]^+$ | adenosine | ASR | OT | 136.06 |
| 20 | 284.0974 | –5.4 | 2.82 | 237.68 | 239.12 | 0.61 | $C_{10}H_{13}N_5O_5$ | $[M+H]^+$ | guanosine or its isomer | ASR | OT | 246.5527, 153.0580, 152.0549 |
| 21 | 266.0884 | –4.2 | 3.03 | 154.24 | 155.20 | 0.62 | $C_{10}H_{13}N_5O_4$ | $[M–H]^–$ | isomer of adenosine | CF | OT | 79.9566 |
| 22 | 625.1403 | –1.2 | 3.35 | 225.58 | 226.38 | 0.35 | $C_{27}H_{30}O_{17}$ | $[M–H]^–$ | isomer of 6-hydroxykaempferol-3,6-di-*O*-*β*-D-glucoside | CF | FL | 625.1402, 491.1182, 314.0413, 298.0466 |
| 23 | 465.1022 | –1.1 | 3.35 | 231.62 | 232.45 | 0.36 | $C_{21}H_{20}O_{12}$ | $[M+H]^+$ | quercetin 6-*O*-*β*-D-glucopyranoside or its isomer | CF | FL | 441.0696, 369.0592, 341.0650, 315.0488 |
| 24 | 299.0764 | –2.9 | 3.58 | 246.05 | 248.50 | 0.99 | $C_{13}H_{16}O_8$ | $[M–H]^–$ | 4-*O*-*β*-D-glucopyranosyl-oxy-benzoic acid or its isomer | CF | OA | 278.0125, 137.0240, 93.0337 |
| 25 | 152.0554 | –8.2 | 3.81 | 121.22 | 121.34 | 0.10 | $C_5H_5N_5O$ | $[M+H]^+$ | guanine or its isomer | ASR | OT | 152.0554, 144.0795, 135.0288, 132.0791 |
| 26 | 609.1456 | –0.8 | 4.22 | 228.29 | 229.74 | 0.63 | $C_{27}H_{30}O_{16}$ | $[M–H]^–$ | kaempferol-3-*O*-*β*-sophorose or its isomer | CF | FL | 489.1032, 437.1079, 299.0555, 135.0444 |
| 27 | 163.0393 | –4.9 | 4.23 | 167.90 | 168.70 | 0.48 | $C_9H_8O_3$ | $[M–H]^–$ | isomer of *p*-coumaric acid | CF | OA | 135.0442, 119.0495, 108.0212 |
| 28 | 351.1650 | 0.1 | 4.50 | | 181.46 | | $C_{15}H_{26}O_9$ | $[M+H]^+$ | eucommioside II or its isomer | SMRR | OT | 308.6464, 260.0978, 216.0995, 163.0379 |
| 29* | 167.0337 | –7.5 | 4.53 | 183.41 | 182.67 | –0.4 | $C_8H_8O_4$ | $[M–H]^–$ | vanillic acid | CR/CF | OA | 167.0337 |
| 30 | 611.1631 | 2.3 | 4.54 | | 317.25 | | $C_{27}H_{32}O_{16}$ | $[M–H]^–$ | (2*S*)-4',5-dihydroxyl-6,7-di-O-β-D-glucopyranosyl flavanone or its isomer | CF | FL | 491.1195, 153.0186, 119.0494 |
| 31 | 515.1404 | –0.4 | 4.64 | 203.50 | 204.55 | 0.52 | $C_{22}H_{28}O_{14}$ | $[M–H]^–$ | isomer of 6,7-dimethoxy-8-hydroxycoumarin 8-*O*-*β*-D | CR | PP | 333.0822, 245.0812, 169.0127 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | -apiofuranosyl-(1→6)-*β*-D-glucopyranoside | | | |
| 32 | 529.2045 | –4.4 | 4.76 | 213.11 | 212.62 | –0.23 | $C_{28}H_{32}O_{10}$ | $[M+H]^+$ | 3"-*O*-(2"'-methylbutyryl)-isoswertisin or its isomer | ASR | FL | 408.1771, 336.0954, 322.0892, 258.1111, 167.0711 |
| 33 | 197.0445 | –5.3 | 4.78 | 186.93 | 185.59 | –0.71 | $C_9H_{10}O_5$ | $[M–H]^–$ | isomer of ethyl gallate | PRR | OA | 182.0208, 166.9967, 145.0291, 123.0083, 95.0133 |
| 34 | 225.0769 | 0.1 | 4.83 | 191.62 | 193.14 | 0.79 | $C_{11}H_{14}O_5$ | $[M–H]^–$ | 4-hydroxy-3,5-dimethoxybenzenepropionic acid or its isomer | CF | OA | 217.0508, 193.0133, 158.0605, 124.0158, |
| 35 | 353.0873 | –1.4 | 4.85 | 168.47 | 168.00 | –0.28 | $C_{16}H_{18}O_9$ | $[M–H]^–$ | neochlorogenic acid or its isomer | CR | OA | 191.0533, 179.0334 |
| 36 | 361.1488 | –4.4 | 4.85 | | 187.66 | | $C_{16}H_{26}O_9$ | $[M–H]^–$ | isomer of 6-*O*-*β*-D-gluecopyranosyl lactinolide | PRR | TP | 272.1052, 203.0852, 97.0183 |
| 37 | 1061.2750 | –2.6 | 4.87 | 298.08 | 300.23 | 0.72 | $C_{48}H_{54}O_{27}$ | $[M–H]^–$ | safflor yellow B or its isomer | CF | FL | 611.1613, 483.0777, 449.1084, 297.0397, 191.0552 |
| 38 | 527.1406 | –0.1 | 4.90 | 202.38 | 201.91 | –0.24 | $C_{23}H_{28}O_{14}$ | $[M–H]^–$ | isomer of 6'-*O*-galloyldesbenzoyl paeoniflorin | PRR | TP | 497.1328, 479.1190, 399.0922, 313.0545 |
| 39 | 141.0556 | 7.3 | 4.90 | 117.28 | 117.51 | 0.20 | $C_7H_8O_3$ | $[M+H]^+$ | 5-hydroxymethylfurfural or its isomer | CR | PL | 141.0555, 127.0529, 117.0560, 89.0372 |
| 40 | 188.0692 | –7.2 | 4.90 | 134.88 | 135.17 | 0.21 | $C_{11}H_9NO_2$ | $[M+H]^+$ | 6-methoxy-4-formyl quinoline or its isomer | SMRR | AL | 154.0637, 143.0713, 118.0635 |
| 41 | 181.0869 | –0.6 | 4.93 | 187.12 | 188.05 | 0.50 | $C_{10}H_{14}O_3$ | $[M–H]^–$ | deoxylpaeonisuffrone or its isomer | PRR | TP | 157.0657, 123.0439, 119.0459, 93.0338 |
| 42 | 627.1563 | 1.1 | 4.94 | 247.37 | 246.64 | –0.29 | $C_{27}H_{30}O_{17}$ | $[M+H]^+$ | 6-hydroxykaempferol-6,7-di-*O*-*β*-D-glucoside or its isomer | CF | FL | 465.1026, 303.0488, 188.0693 |
| 43 | 801.1744 | 1.6 | 4.94 | 281.34 | 281.60 | 0.09 | $C_{33}H_{38}O_{23}$ | $[M–H]^–$ | 6-hydroxykaempferol-3,6-di-*O*-*β*-D-glucoside-7-*O*-*β*-D-glucuronide or its isomer | CF | FL | 787.1942, 625.1407, 463.0874, 301.0343 |
| 44 | 343.1393 | –1.5 | 4.95 | 184.90 | 182.67 | –1.21 | $C_{16}H_{24}O_8$ | $[M–H]^–$ | mudanpioside F or its isomer | PRR | TP | 289.0706, 245.0812, 203.0698, 151.0395, 119.0495 |
| 45 | 449.1085 | 1.6 | 4.95 | 240.44 | 242.69 | 0.94 | $C_{21}H_{20}O_{11}$ | $[M+H]^+$ | carthamone or its isomer | CF | FL | 371.0787, 303.0488, 188.0693, 146.0585 |
| 46 | 771.1970 | –2.6 | 4.97 | | 268.61 | | $C_{33}H_{40}O_{21}$ | $[M–H]^–$ | 6-hydroxykaempferol-3-*O*-*β*-rutinoside-6-*O*-*β*-D-glucoside or its isomer | CF | FL | 609.1461,463.0873, 301.0342, 271.0237 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 47* | 787.1942 | 0.4 | 4.97 | | 285.21 | | $C_{33}H_{40}O_{22}$ | $[M–H]^-$ | quercetin-3-O-β-D-glucose-7-O-β-D-gentiobioside | CF | FL | 625.1407, 463.0874 |
| 48 | 515.1388 | –3.5 | 5.02 | 206.18 | 205.60 | –0.28 | $C_{22}H_{28}O_{14}$ | $[M–H]^-$ | isomer of 6,7-dimethoxy-8-hydroxycoumarin 8-*O*-*β*-D-apiofuranosyl-(1→6)-*β*-D-glucopyranoside | CR | PP | 449.1082, 345.1117, 215.0330, 191.0574, 159.0442 |
| 49 | 413.1958 | 0.0 | 5.02 | | 192.88 | | $C_{24}H_{28}O_6$ | $[M+H]^+$ | isomer of chuanxiongnolide L4 | CR | PL | 395.5662, 304.0519, 232.0993, 108.0436 |
| 50 | 443.1909 | –3.0 | 5.11 | 193.87 | 194.85 | 0.51 | $C_{21}H_{32}O_{10}$ | $[M–H]^-$ | isomer of dihydrophaseic methyl-4'-*O*-*β*-D-glucoside | CF | OT | 323.0542, 211.0232, 175.0396 |
| 51 | 415.1014 | –2.3 | 5.14 | 197.46 | 196.74 | –0.36 | $C_{21}H_{18}O_9$ | $[M+H]^+$ | isomer of saffloflavoneside A | CF | FL | 313.0683, 277.0330, 247.0223, 235.0221, 147.0427 |
| 52 | 451.1228 | –1.6 | 5.14 | 204.42 | 204.98 | 0.27 | $C_{21}H_{22}O_{11}$ | $[M+H]^+$ | 5,6,7,4'-rahydroxyflavanone-5-*O*-*β*-D-glucoside or its isomer | CF | FL | 379.0909, 367.0803, 313.0683, 211, 0221, 193.0117 |
| 53 | 595.1659 | 0.3 | 5.14 | 241.26 | 243.22 | 0.81 | $C_{27}H_{30}O_{15}$ | $[M+H]^+$ | isomer of safflor yellow A | CF | FL | 433.1124, 415.1015, 397.0906, 379.0805, 331.0804 |
| 54* | 611.1611 | 1.0 | 5.15 | 238.59 | 240.42 | 0.77 | $C_{27}H_{32}O_{16}$ | $[M–H]^-$ | hydroxysafflor yellow A | CF | FL | 491.1186, 325.0705, 283.0596, 119.0494 |
| 55 | 625.1406 | –0.7 | 5.19 | 249.45 | 252.17 | 1.09 | $C_{27}H_{30}O_{17}$ | $[M–H]^-$ | isomer of 6-hydroxykaempferol-3,6-di-*O*-*β*-D-glucoside | CF | FL | 463.0877, 301.0264, 271.0200 |
| 56 | 179.0348 | –1.1 | 5.20 | 178.21 | 178.72 | 0.29 | $C_9H_8O_4$ | $[M–H]^-$ | isomer of caffeic acid | ASR | OA | 179.0337, 170.0617, 135.0443 |
| 57 | 609.1467 | 1.0 | 5.21 | 238.54 | 239.47 | 0.39 | $C_{27}H_{30}O_{16}$ | $[M–H]^-$ | kaempferol-3-*O*-*β*-D-glucoside-7-*O*-*β*-D-glucuronide or its isomer | CF | FL | 463, 0877, 301.0342, 271.0237, 253.0863, 165.9900 |
| 58 | 527.1398 | –1.5 | 5.23 | 200.48 | 200.01 | –0.23 | $C_{23}H_{28}O_{14}$ | $[M–H]^-$ | 8-*O*-galloyldebenzoyl paeoniflorin or its isomer | PRR | TP | 465.1396, 437.1085, 299.0550, 231.0763, 137.0234 |
| 59* | 495.1501 | –1.5 | 5.23 | 198.72 | 199.25 | 0.27 | $C_{23}H_{28}O_{12}$ | $[M–H]^-$ | oxypaeoniflorin | PRR | TP | 465.1396, 437.1085, 137.0234, 93.0338 |
| 60 | 333.0973 | –1.9 | 5.23 | 197.05 | 199.41 | 1.20 | $C_{17}H_{18}O_7$ | $[M–H]^-$ | isomer of 4'-hydroxypaeoniflorigenone | PRR | TP | 177.0551, 165.0545, 149.0603, 137.0234, 93.0338 |

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| 61 | 223.0600 | –5.3 | 5.27 | 203.55 | 202.96 | –0.29 | $C_{11}H_{12}O_5$ | $[M–H]^-$ | sinapic acid or its isomer | CF | OA | 187.0398, 177.0551, 137.0234, 93.0338 |
| 62 | 521.0945 | 1.7 | 5.30 | 214.63 | 215.49 | 0.40 | $C_{23}H_{22}O_{14}$ | $[M–H]^-$ | isomer of quercetin-7-*O*-(6-*O*-acetyl)-*β*-D-glucopyranoside | CF | FL | 519.1130, 449.1083, 311.0573, 243.0656 |
| 63* | 289.0710 | –2.8 | 5.32 | 155.67 | 156.37 | 0.45 | $C_{15}H_{14}O_6$ | $[M–H]^-$ | catechin | PRR | FL | 289.0706, 271.0229 |
| 64 | 445.2201 | –4.5 | 5.32 | 196.95 | 198.15 | 0.61 | $C_{25}H_{32}O_7$ | $[M+H]^+$ | angesinenolides B or its isomer | ASR | OT | 376.1025, 373.0489, 343.1635, 189.0720 |
| 65 | 511.1454 | –0.6 | 5.35 | 262.94 | 264.16 | 0.46 | $C_{23}H_{28}O_{13}$ | $[M–H]^-$ | isomer of mudanpioside E | PRR | TP | 449.1080, 289.0706, 179.0345, 173.0451 |
| 66* | 353.0872 | –1.8 | 5.35 | | 256.62 | | $C_{16}H_{18}O_9$ | $[M–H]^-$ | chlorogenic acid | CF | OA | 179.0343, 135.0440 |
| 67 | 623.1263 | 1.6 | 5.36 | 227.33 | 230.94 | 1.59 | $C_{27}H_{28}O_{17}$ | $[M–H]^-$ | isomer of 6-hydroxyapigenin -6-*O*-*β*-D-glucoside-7-*O*-*β*-D-glucuronide | CF | FL | 611.1615, 385.0921, 335.0814, 205.0136, 119.0495 |
| 68 | 193.0480 | –7.8 | 5.38 | 128.67 | 128.34 | –0.25 | $C_{10}H_8O_4$ | $[M+H]^+$ | 3-carboxyrthyl-phthalide or its isomer | CR | PL | 178.0247, 140.0488, 133.0269, 115.0523 |
| 69 | 191.0340 | –4.9 | 5.39 | 223.80 | 222.97 | –0.37 | $C_{10}H_8O_4$ | $[M–H]^-$ | isomer of scopoletin | CR | OT | 176.0108, 169.0135, 161.0242, 125.0235 |
| 70* | 183.0298 | –0.8 | 5.40 | 128.58 | 128.74 | 0.13 | $C_8H_8O_5$ | $[M–H]^-$ | methyl gallate | PRR | OA | 183.0298, 177.0182, 135.0446 |
| 71 | 635.0894 | 0.6 | 5.43 | 222.94 | 220.82 | –0.95 | $C_{27}H_{24}O_{18}$ | $[M–H]^-$ | gallotannin or its isomer | PRR | OT | 597.1553, 463.2187, 301.0347, 169.0135, 125.0235 |
| 72 | 283.1665 | –1.1 | 5.45 | | 165.82 | | $C_{17}H_{24}O_2$ | $[M+Na]^+$ | (3*R*,8*R*,9*Z*)-1,9-heptadecadiene-4,6-diyne-3,8-diol or its isomer | ASR | OT | 271.0591, 229.0492, 206.0825, 192.0648, 136.0740 |
| 73 | 449.1082 | 0.9 | 5.45 | | 244.44 | | $C_{21}H_{20}O_{11}$ | $[M+H]^+$ | isomer of luteolin-7-*O*-*β*-D-glucopyranoside | SMRR | FL | 381.0988, 319.0470, 287.0538, 217.0955, 144.0790 |
| 74 | 593.1516 | 0.6 | 5.48 | | 232.24 | | $C_{27}H_{30}O_{15}$ | $[M–H]^-$ | isomer of kaempferol-3-*O*-*α*-l-rhamnopyranosyl-(1→6)-*β*-D-glucopyranoside | SMRR | FL | 575.1346, 491.1189, 328.0587, 271.0239, 215.0707 |
| 75 | 787.1967 | 3.7 | 5.51 | 265.52 | 264.90 | 0.48 | $C_{33}H_{40}O_{22}$ | $[M–H]^-$ | 6-hydroxykaempferol-3,6,7-tri-*O*-*β*-D-glucoside or its isomer | CF | FL | 625.1416, 463.0876, 301.0345 |

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| 76 | 611.1619 | 0.2 | 5.62 | 238.45 | 239.62 | 0.49 | $C_{27}H_{32}O_{16}$ | $[M–H]^-$ | saffloquinoside D or its isomer | CF | FL | 431.0992, 403.1038, 313.0716, 145.0291, 119.0495 |
| 77 | 387.1657 | –1.0 | 5.64 | 184.59 | 184.08 | –0.28 | $C_{18}H_{28}O_9$ | $[M–H]^-$ | isomer of chuanxiongoside A | CR | PL | 387.1656, 171.0442 |
| 78* | 179.0342 | –4.2 | 5.73 | | 130.79 | | $C_9H_8O_4$ | $[M–H]^-$ | caffeic acid | CF | OA | 135.0448 |
| 79 | 577.1574 | 2.0 | 5.77 | | 240.04 | | $C_{27}H_{30}O_{14}$ | $[M–H]^-$ | isomer of 5,7-dihydroxy-4'-methoxyflavone 7-*O*-*β*-D-apiofuranosyl-(1-6)-*O*-*β*-D-glucoside | CF | FL | 471.0951, 301.0307, 135.0448 |
| 80 | 497.1618 | –2.3 | 5.84 | | 210.80 | | $C_{21}H_{30}O_{12}$ | $[M+Na]^+$ | 3-hydroxy-4-methoxypropiophenone 3-*O*-*β*-D-apiofuranosyl-(1→6)-*β*-D-glucopyranoside or its isomer | CR | PP | 477.2304, 413.0522 |
| 81 | 399.1586 | 4.8 | 5.86 | | 186.79 | | $C_{24}H_{24}O_4$ | $[M+Na]^+$ | isomer of *Z*,*Z*′-3.3'8.8'-diligustilide | ASR | PL | 377.1443, 250.1171, 243.0863, 191.0688, 172.0853 |
| 82 | 197.1287 | –4.5 | 5.87 | 157.93 | 157.60 | –0.21 | $C_{10}H_{18}N_2O_2$ | $[M–H]^-$ | L-isobutyl-L-valine anhydride or its isomer | CR | AL | 197.1287 |
| 83 | 1043.2680 | 0.7 | 5.87 | 325.88 | 326.67 | 0.24 | $C_{48}H_{52}O_{26}$ | $[M–H]^-$ | isomer of anhydrosafflor yellow B | CF | FL | 595.1542, 559.1216, 407.0970, 333.0795 |
| 84 | 377.1448 | 1.4 | 5.90 | 182.42 | 183.49 | 0.59 | $C_{16}H_{24}O_{10}$ | $[M+H]^+$ | isomer of desbenzoylpaeoniflorin | PRR | TP | 377.1443, 321.6131, 250.1171, 191.0688, 172.0853 |
| 85 | 503.1755 | –3.1 | 5.94 | 211.87 | 208.00 | –1.83 | $C_{22}H_{32}O_{13}$ | $[M–H]^-$ | 3,5-dimethoxy-4-hydroxypropiophenone 4-*O*-*β*-D-apiofuranosyl-(1→6)-*β*-D-glucopyranoside or its isomer | CR | PP | 273.0375, 215.0705, 167.0705, 134.0371 |
| 86 | 593.1511 | –0.1 | 5.94 | 232.05 | 236.40 | 1.88 | $C_{27}H_{30}O_{15}$ | $[M–H]^-$ | isomer of kaempferol-3-*O*-*α*-l-rhamnopyranosyl-(1→6)-*β*-d-glucopyranoside | SMRR | FL | 575.1394, 443.0982, 301.0694, 289.0704, 268.0681 |
| 87 | 771.1986 | –0.4 | 6.02 | 257.23 | 255.05 | –0.85 | $C_{33}H_{40}O_{21}$ | $[M–H]^-$ | isomer of 6-hydroxykaempferol-3-*O*-*β*-rutinoside-6-*O*-*β*-D-glucoside | CF | FL | 609.1455, 463.0882, 301.0341, 271.0238 |

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| 88 | 329.1589 | –1.8 | 6.05 | 170.75 | 171.02 | 0.16 | $C_{16}H_{24}O_7$ | $[M+H]^+$ | (8*S*)-deca-4,6-diyne-1,8-diol-8-*O*-*β*-D-glucopyranoside or its isomer | CF | OT | 247.0266, 191.0685, 169.0643, 136.0604, 115.0527 |
| 89 | 269.1018 | –4.6 | 6.05 | 206.04 | 207.03 | 0.48 | $C_{13}H_{18}O_6$ | $[M–H]^–$ | benzyl-*O*-*β*-D-glucopyranoside or its isomer | CF | OT | 191.0555, 179.0341, 161.0605, 135.0438 |
| 90 | 625.1409 | –0.2 | 6.21 | 246.17 | 245.95 | –0.09 | $C_{27}H_{30}O_{17}$ | $[M–H]^–$ | isomer of 6-hydroxykaempferol-3,6-di-*O*-*β*-D-glucoside | CF | FL | 625, 1403, 463.0870, 301.0338, 271.0236 |
| 91 | 319.0441 | –2.2 | 6.22 | 201.86 | 202.01 | 0.08 | $C_{15}H_{10}O_8$ | $[M+H]^+$ | isomer of myricetin | CF | FL | 303.0485, 273.0377, 99.0426 |
| 92 | 669.2399 | –0.1 | 6.31 | 236.60 | 238.25 | 0.70 | $C_{31}H_{42}O_{16}$ | $[M–H]^–$ | isomer of chuanxiongoside A | CR | PP | 669.2392, 591.2671, 491.1186, 312.0986, 135.0449 |
| 93 | 647.1618 | 0.0 | 6.33 | 229.98 | 229.62 | –0.16 | $C_{30}H_{32}O_{16}$ | $[M–H]^–$ | isomer of galloyloxypaeoniflorin | PRR | TP | 629.1509, 509.1303, 491.1186, 313.0558, 211.0238 |
| 94 | 317.1050 | 6.1 | 6.38 | 213.28 | 211.22 | –0.97 | $C_{17}H_{18}O_6$ | $[M–H]^–$ | paeoniflorigenone or its isomer | PRR | TP | 312.0986, 149.0239, 121.0290, 77.0389 |
| 95 | 479.1560 | 0.2 | 6.39 | 212.42 | 212.30 | –0.06 | $C_{23}H_{28}O_{11}$ | $[M–H]^–$ | albiflorin or its isomer | PRR | TP | 327.1223, 312.0986, 149.0239, 121.0290, 77.0389 |
| 96 | 197.0792 | –8.1 | 6.39 | 210.10 | 211.34 | 0.59 | $C_{10}H_{12}O_4$ | $[M+H]^+$ | isomer of paeonilactone B | PRR | TP | 161.0592, 105.0318, 77.0365 |
| 97 | 641.2088 | 0.2 | 6.40 | 246.33 | 245.32 | –0.41 | $C_{29}H_{38}O_{16}$ | $[M–H]^–$ | *β*-gentiobiosylpaeoniflorin or its isomer | PRR | TP | 519.1708, 489.1627, 245.0448, 77.0390 |
| 98 | 507.1922 | 9.9 | 6.41 | 220.46 | 218.79 | –0.76 | $C_{25}H_{32}O_{11}$ | $[M–H]^–$ | 4-ethyl-paeoniflorin or its isomer | PRR | TP | 327.1223, 312.0986, 241.0494, 121.0290 |
| 99 | 613.1579 | 2.7 | 6.42 | 227.17 | 231.33 | 1.83 | $C_{30}H_{30}O_{14}$ | $[M–H]^–$ | saffloquinoside E or its isomer | CF | FL | 581.1523, 407.0982, 287.0543, 241.0494 |
| 100 | 623.1252 | –0.2 | 6.46 | 245.52 | 246.00 | 0.20 | $C_{27}H_{28}O_{17}$ | $[M–H]^–$ | quercetin-3-*O*-*α*-L-rhamnoside-7-*O*-*β*-D-glucuronide or its isomer | CF | FL | 447.0926, 385.0920, 285.0393, 267.0655 |
| 101 | 611.1611 | –1.0 | 6.47 | | 238.09 | | $C_{27}H_{32}O_{16}$ | $[M–H]^–$ | isomer of HSYA | CF | FL | 491.1194, 325.0712, 283.0236, 119.0495 |
| 102 | 609.1453 | –1.3 | 6.51 | 242.14 | 242.22 | 0.03 | $C_{27}H_{30}O_{16}$ | $[M–H]^–$ | kaempferol-3-*O*-*β*-sophorose or its isomer | CF | FL | 521.1293, 447.0926, 313.0694, 285.0393, 255.0291 |
| 103 | 669.2399 | –0.2 | 6.53 | 235.41 | 236.87 | 0.62 | $C_{31}H_{42}O_{16}$ | $[M–H]^–$ | isomer of chuanxiongoside A | CR | PP | 611.1611, 491.1194, 313.0694, 255.0291 |
| 104 | 577.1542 | –3.6 | 6.61 | 219.92 | 222.88 | 1.33 | $C_{27}H_{30}O_{14}$ | $[M–H]^–$ | 5,7-dihydroxy-4'-methoxyflavone 7-*O*-*β*-D-apiofuranosyl-(1-6)-*O*-*β*-D-glucoside or its | CF | FL | 563.1405, 463.2174, 313.0565, 169.0132 |

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| | | | | | | | | | isomer | | | |
| 105 | 357.0627 | 3.2 | 6.61 | 172.64 | 173.84 | 0.60 | $C_{18}H_{14}O_8$ | $[M–H]^-$ | prolithospermic acid or its isomer | SMRR | OA | 357.0627, 345.0972, 313.0704, 269.0808 |
| 106 | 1087.2580 | 0.3 | 6.70 | 298.35 | 298.44 | 0.03 | $C_{49}H_{52}O_{28}$ | $[M–H]^-$ | isomer of carthorquinoside A | CF | FL | 625.1419, 461.1064, 449.1089, 271.0595 |
| 107 | 339.1242 | 1.1 | 6.75 | 262.90 | 264.48 | 0.60 | $C_{20}H_{20}O_5$ | $[M–H]^-$ | isomer of chuanxiongnolide L3 | CR | PL | 324.0984, 309.0758, 301.0709, 213.0546, 161.0238 |
| 108 | 941.3092 | 0.8 | 6.89 | 299.08 | 300.80 | 0.58 | $C_{46}H_{54}O_{21}$ | $[M–H]^-$ | isomer of paeonidanin E | PRR | TP | 449.1448, 327.1087, 165.0548, 121.0287 |
| 109 | 479.1555 | –0.8 | 6.93 | 215.01 | 216.29 | 0.59 | $C_{23}H_{28}O_{11}$ | $[M–H]^-$ | paeoniflorin or its isomer | PRR | TP | 449.1448, 327.1078, 165.0548, 121.0287 |
| 110 | 1087.2500 | –6.7 | 6.97 | 306.58 | 312.68 | 1.99 | $C_{49}H_{52}O_{28}$ | $[M–H]^-$ | isomer of carthorquinoside A | CF | FL | 625.1402, 591.2654, 449.1394 |
| 111 | 121.0286 | –7.2 | 6.99 | 222.82 | 224.34 | 0.68 | $C_7H_6O_2$ | $[M–H]^-$ | isomer of benzoic acid | PRR | OA | 85.0289, 78.0417, 77.0389 |
| 112 | 313.0713 | –1.4 | 7.01 | | 260.89 | | $C_{17}H_{14}O_6$ | $[M–H]^-$ | salvianolic acid F or its isomer | SMRR | OA | 269.0806, 255.0662 |
| 113 | 163.0393 | –4.7 | 7.04 | 173.23 | 173.19 | –0.02 | $C_9H_8O_3$ | $[M–H]^-$ | isomer of *p*-coumaric acid | CF | OA | 119.0494, 117.0343 |
| 114 | 325.0922 | –2.0 | 7.04 | 169.50 | 170.91 | 0.83 | $C_{15}H_{18}O_8$ | $[M–H]^-$ | isomer of 4-*O*-*β*-D-glucosyl-*cis*-*p*-coumaric acid | CF | OA | 269.0813, 254.0575, 253.0497, 119.0494 |
| 115 | 445.1723 | 1.7 | 7.05 | 205.87 | 209.08 | 1.56 | $C_{20}H_{30}O_{11}$ | $[M–H]^-$ | 2-phenylethyl[-*β*-D-glucopyranosyl-(1→6)]-*β*-D-glucopyranoside or its isomer | PRR | OT | 363.0670, 327.0496, 269.0449, 203.0731 |
| 116 | 135.0448 | –2.8 | 7.07 | 120.37 | 121.48 | 0.92 | $C_8H_8O_2$ | $[M–H]^-$ | p-hydroxyacetophenone or its isomer | CF | OT | 135.0448, 93.0338 |
| 117 | 309.1318 | –4.9 | 7.15 | 167.68 | 167.68 | 0.00 | $C_{16}H_{20}O_6$ | $[M+H]^+$ | 4,6,8-dec-atriyne-1-*O*-*β*-D-glucopyranoside or its isomer | CF | OT | 287.0536, 269.0433, 169.0121 |
| 118 | 415.1237 | –2.1 | 7.17 | 196.21 | 197.20 | 0.51 | $C_{18}H_{24}O_{11}$ | $[M–H]^-$ | 2-*O*-[*α*-L-arabinopyranosyl-(1→6)-*β*-D-glucopyranoside]-Benzaldehyde or its isomer | PRR | TP | 407.0994, 231.0297, 221.1068 |
| 119 | 303.0484 | –5.1 | 7.21 | 230.57 | 232.49 | 0.84 | $C_{15}H_{10}O_7$ | $[M+H]^+$ | isomer of 6-Hydroxykaempferol | CF | FL | 274.0474, 257.0438, 229.0481, 169.0121 |
| 120 | 609.1456 | –0.8 | 7.22 | 241.50 | 243.89 | 0.99 | $C_{27}H_{30}O_{16}$ | $[M–H]^-$ | kaempferol-3-*O*-*β*-D-glucoside-7-*O*-*β*-D-glucuronide or its isomer | CF | FL | 301.0342, 271.0238, 165.9897 |
| 121 | 1043.2680 | 0.7 | 7.26 | 316.97 | 318.91 | 0.61 | $C_{48}H_{52}O_{26}$ | $[M–H]^-$ | isomer of anhydrosafflor yellow B | CF | FL | 1025.2558, 923.2266, 607.1317, 501.1619, 301.0704 |

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| 122 | 169.0133 | –5.7 | 7.35 | 154.92 | 155.21 | 0.19 | $C_7H_6O_5$ | $[M–H]^-$ | isomer of gallic acid | PRR | OA | 169.0133, 135.0451 |
| 123 | 593.1509 | –0.5 | 7.40 | 233.35 | 236.97 | 1.55 | $C_{27}H_{30}O_{15}$ | $[M–H]^-$ | saffloquinoside C or its isomer | CF | FL | 521.1291, 445.1154, 295.0593, 169.0135 |
| 124 | 495.1503 | –1.1 | 7.41 | 202.80 | 204.11 | 0.65 | $C_{23}H_{28}O_{12}$ | $[M–H]^-$ | isomer of oxypaeoniflorin | PRR | TP | 465.1408, 308.1148, 137.0234, 93.0339 |
| 125 * | 197.0448 | –4.0 | 7.42 | 136.36 | 137.14 | 0.57 | $C_9H_{10}O_5$ | $[M–H]^-$ | ethyl gallate | PRR | OA | 124.0156 |
| 126 | 397.1845 | –5.7 | 7.43 | 232.99 | 237.16 | 1.79 | $C_{20}H_{30}O_8$ | $[M–H]^-$ | (2*E*)-tetradecaene-4,6-diyne-1,10,14-triol-1-*O*-*β*-D-glucopyranoside or its isomer | CF | OT | 333.0803, 313.0570, 187.0391 |
| 127 | 413.0869 | –2.1 | 7.44 | 197.14 | 197.19 | 0.02 | $C_{21}H_{18}O_9$ | $[M–H]^-$ | isomer of saffloflavonesides A | CF | FL | 353.0659, 137.0233, 93.0339 |
| 128 | 137.0236 | –5.7 | 7.46 | 208.90 | 211.87 | 1.42 | $C_7H_6O_3$ | $[M–H]^-$ | protocatechualdehyde or its isomer | PRR | TP | 137.0234, 94.0370, 93.0339 |
| 129 | 609.1461 | 0.0 | 7.52 | 240.57 | 238.38 | –0.91 | $C_{27}H_{30}O_{16}$ | $[M–H]^-$ | isomer of kaempferol-3-*O*-*β*-D-glucoside-7-*O*-*β*-D-glucuronide | CF | FL | 447.0922, 285.0381, 227.0339, 151.0029 |
| 130 | 301.0347 | –2.3 | 7.64 | 197.55 | 197.10 | –0.23 | $C_{15}H_{10}O_7$ | $[M–H]^-$ | isomer of 6-hydroxykaempferol | CF | FL | 271.0237, 243.0288, 165.9901, 139.0031 |
| 131 | 611.1614 | –0.5 | 7.66 | | 241.95 | | $C_{27}H_{30}O_{16}$ | $[M–H]^-$ | saffloquinoside D or its isomer | CF | FL | 449.1079, 287.0551, 153.0186 |
| 132 | 271.0608 | –1.4 | 7.75 | 200.98 | 202.88 | 0.94 | $C_{15}H_{12}O_5$ | $[M–H]^-$ | isomer of naringenin | PRR | FL | 271.0595 |
| 133 | 521.0930 | –1.3 | 7.92 | 211.62 | 212.88 | 0.60 | $C_{23}H_{22}O_{14}$ | $[M–H]^-$ | quercetin-7-*O*-(6-*O*-acetyl)-*β*-D-glucopyranoside or its isomer | CF | FL | 477.1035, 315.0498, 286.0469, 257.0455 |
| 134 | 425.1444 | 6.1 | 8.02 | | 176.43 | | $C_{18}H_{26}O_{10}$ | $[M+Na]^+$ | methyl syrigin or its isomer | SMRR | PP | 355.1717, 353.1560, 337.1821, 216.9784 |
| 135 | 265.1036 | –4.1 | 8.06 | | 163.82 | | $C_{12}H_{18}O_5$ | $[M+Na]^+$ | 3-hydroxy-4,5,6,7-tetrahydro-6,7-dihydroxy-3-butylphthalide or its isomer | CR | PL | 169.0124, 115.0527 |
| 136 | 595.1659 | 0.3 | 8.08 | 230.30 | 233.13 | 1.23 | $C_{27}H_{30}O_{15}$ | $[M+H]^+$ | isomer of kaempferol-3-*O*-*β*-rutinoside | CF | FL | 563.2072, 395.0426, 303.0497, 208.0581 |
| 137 | 193.0486 | –5.1 | 8.24 | 128.93 | 128.64 | –0.23 | $C_{10}H_8O_4$ | $[M+H]^+$ | isomer of scopoletin | CR | OT | 178.0256, 150.0307, 133.0269, 122.0344 |
| 138 | 313.0713 | –1.6 | 8.30 | | 204.51 | | $C_{17}H_{14}O_6$ | $[M–H]^-$ | isomer of salvianolic acid F | SMRR | OA | 175.0387 |
| 139 | 371.0948 | –6.5 | 8.33 | | 178.44 | | $C_{16}H_{18}O_{10}$ | $[M+H]^+$ | isomer of isofraxoside | CR | PP | 353.1198, 223.0054, 207.9806, 192.9566 |
| 140 | 271.0611 | –0.4 | 8.35 | 199.65 | 199.30 | –0.18 | $C_{15}H_{12}O_5$ | $[M–H]^-$ | isomer of naringenin | PRR | FL | 271.0598, 222.9244, 151.0027, 119.0490 |
| 141 | 193.0498 | –4.4 | 8.39 | | 136.68 | | $C_{10}H_{10}O_4$ | $[M–H]^-$ | ferulic acid | CF | OA | 193.0498 |

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| 142 | 311.1477 | –3.8 | 8.42 | 171.28 | 172.56 | 0.74 | $C_{16}H_{22}O_6$ | $[M+H]^+$ | (8E)-decaene-4,6-diyne- 1-*O*-*β*-D-glucopyranoside or its isomer | CF | OT | 216.9788, 191.1061, 149.0583, 115.0529, 91.0524 |
| 143 | 287.0551 | –3.4 | 8.48 | 187.27 | 188.71 | 0.77 | $C_{15}H_{12}O_6$ | $[M–H]^–$ | isomer of (-)-eriodictyol | CF | OT | 181.0132, 166.9978, 153.0183, 139.0028, 136.9896 |
| 144 * | 609.1457 | –0.6 | 8.56 | 229.57 | 233.03 | 1.51 | $C_{27}H_{30}O_{16}$ | $[M–H]^–$ | rutin | CF | FL | 301.0263, 271.0235, 151.0027 |
| 145 | 373.1465 | –1.1 | 8.66 | | 180.98 | | $C_{15}H_{26}O_9$ | $[M+Na]^+$ | eucommioside II or its isomer | SMRR | OT | 361.1768, 355.1709, 229.1195 |
| 146 | 503.2129 | –0.9 | 8.91 | 221.15 | 221.56 | 0.18 | $C_{23}H_{36}O_{12}$ | $[M–H]^–$ | isomer of ligusticoside B | CR | PL | 285.039 |
| 147 | 576.1712 | 0.1 | 8.94 | 237.90 | 240.55 | 1.11 | $C_{27}H_{29}NO_{13}$ | $[M+H]^+$ | cartormine or its isomer | CF | FL | 559.1467, 414.1208, 356.9693, 289.0695, 246.0382 |
| 148 | 592.1672 | 0.0 | 8.96 | 237.18 | 239.19 | 0.85 | $C_{27}H_{31}NO_{14}$ | $[M–H]^–$ | tinctormine or its isomer | CF | FL | 472.1087, 364.0820, 285.0382, 233.0314, 216.0278 |
| 149 | 303.0490 | –6.6 | 8.99 | 162.50 | 163.14 | 0.39 | $C_{15}H_{12}O_7$ | $[M–H]^–$ | dihydroquercetin or its isomer | PRR | FL | 303.0490, 285.0396, 259.1535 |
| 150 | 503.2130 | –0.9 | 9.16 | 222.21 | 222.91 | 0.32 | $C_{23}H_{36}O_{12}$ | $[M–H]^–$ | chuanxiongoside B or its isomer | CR | PL | 451.3277, 287.0522, 183.1012, 153.0183 |
| 151 * | 463.0878 | –0.8 | 9.17 | 198.26 | 198.91 | 0.33 | $C_{21}H_{20}O_{12}$ | $[M–H]^–$ | hyperoside | CF | FL | 300.0267, 271.0239, 255.0288, 243.0286, 151.0033 |
| 152 | 411.1669 | 4.7 | 9.17 | | 141.50 | | $C_{20}H_{26}O_9$ | $[M+H]^+$ | 3-*O*-caffeoylquinic acid butyl ester or its isomer | SMRR | OA | 249.0415, 233.0687, 129.0674, 91.0524 |
| 153 | 447.0931 | –0.5 | 9.20 | 203.58 | 203.14 | –0.22 | $C_{21}H_{20}O_{11}$ | $[M–H]^–$ | isomer of luteolin-7-*O*-*β*-D-glucopyranoside | CF | FL | 285.0392 |
| 154 | 223.0950 | –6.8 | 9.57 | 149.32 | 149.60 | 0.19 | $C_{12}H_{14}O_4$ | $[M+H]^+$ | 4,7-dihydroxy-3-butylphthalide or its isomer | CR | PL | 223.0739, 205.0653, 176.0610, 167.0707, 151.0531 |
| 155 * | 447.0930 | –0.7 | 9.63 | 198.68 | 199.17 | 0.24 | $C_{21}H_{20}O_{11}$ | $[M–H]^–$ | kaempferol-3-*O*-*β*-D-glucoside | CF | FL | 301.0342, 243.0289 |
| 156 | 631.1676 | 1.1 | 9.71 | 223.48 | 221.89 | –0.71 | $C_{30}H_{32}O_{15}$ | $[M–H]^–$ | isomer of galloylpaeoniflorin | PRR | TP | 613.1560, 491.1189, 399.0924, 271.0450, 121.0288 |

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| 157 | 289.0693 | –4.7 | 9.79 | 160.09 | 160.45 | 0.22 | $C_{15}H_{12}O_6$ | $[M+H]^+$ | isomer of (-)–eriodictyol | CF | OT | 169.0115, 147.0428, 119.0480 |
| 158 | 369.1508 | –9.8 | 9.88 | | 183.52 | | $C_{18}H_{24}O_8$ | $[M+H]^+$ | isomer of celephthalide A | CR | PL | 217.1784, 221.0245, 216.1734, 160.1110, 144.0797 |
| 159 | 609.1469 | 1.2 | 10.01 | 231.03 | 234.10 | 1.33 | $C_{27}H_{30}O_{16}$ | $[M–H]^–$ | isomer of rutin | CF | FL | 301.0343, 271.0238, 151.0025 |
| 160 | 233.1179 | –1.7 | 10.02 | 209.26 | 210.91 | 0.79 | $C_{14}H_{18}O_3$ | $[M–H]^–$ | (2E,8E)-tetradecadiene-4,6-diyne-1,11,14-triol or its isomer | CF | OT | 161.0237, 136.0489 |
| 161 | 343.1394 | 1.8 | 10.18 | | 128.15 | | $C_{16}H_{22}O_8$ | $[M+H]^+$ | methyl-3-(4-*O*-*β*-D-glucopyranosylphenyl) propionate or its isomer | CF | OT | 313.1399, 249.0413, 233.0687, 145.0160, 139.0508 |
| 162 | 939.1115 | 0.6 | 10.31 | 290.21 | 294.34 | 1.42 | $C_{41}H_{32}O_{26}$ | $[M–H]^–$ | 1,2,3,4,6-*O*-pentagalloylglucose or its isomer | PRR | OT | 769.0901, 617.0793, 465.0699, 311.0551, 229.0503 |
| 163 | 209.1159 | –6.5 | 10.35 | 157.33 | 157.65 | 0.20 | $C_{12}H_{16}O_3$ | $[M+H]^+$ | senkyunolide H or its isomer | CR | PL | 203.0730, 191.1052, 162.9831, 149.0580, 121.0634 |
| 164 | 227.1268 | –4.3 | 10.35 | 157.68 | 159.29 | 1.02 | $C_{12}H_{18}O_4$ | $[M+H]^+$ | senkyunolide J/N or its isomer | CR | PL | 203.0730, 218.1172, 191.1052, 163.1102 |
| 165* | 1043.2680 | 0.1 | 10.37 | 341.28 | 341.92 | 1.87 | $C_{48}H_{52}O_{26}$ | $[M–H]^–$ | anhydrosafflor yellow B | CF | FL | 1025.2564, 923.2247, 862.1965, 772.1656 |
| 166 | 647.1611 | –1.0 | 10.37 | 225.84 | 225.69 | –0.07 | $C_{30}H_{32}O_{16}$ | $[M–H]^–$ | galloyloxypaeoniflorin or its isomer | PRR | TP | 632.1647, 449.1049, 399.0935, 211.0233 |
| 167 | 295.0606 | –1.9 | 10.58 | 212.39 | 211.56 | –0.39 | $C_{17}H_{12}O_5$ | $[M–H]^–$ | isomer of miltiolignanolides A | SMRR | TP | 210.0325, 186.0307, 137.0234, 125.0236 |
| 168 | 339.0502 | –2.4 | 10.58 | 212.99 | 212.38 | –0.29 | $C_{18}H_{12}O_7$ | $[M–H]^–$ | isomer of miltiolignanolides C | SMRR | TP | 224.0460, 210.0325, 186.0307, 137.0234, 125.0236 |
| 169 | 449.1072 | –1.4 | 10.60 | | 229.30 | | $C_{21}H_{20}O_{11}$ | $[M+H]^+$ | isomer of luteolin-7-*O*-*β*-D-glucopyranoside | SMRR | FL | 287.0535, 153.0166 |
| 170 | 593.1515 | 0.5 | 10.62 | | 228.23 | | $C_{27}H_{30}O_{15}$ | $[M–H]^–$ | isomer of kaempferol-3-*O*-*α*-l-rhamnopyranosyl-(1→6)-*β*-d-glucopyranoside | SMRR | FL | 593.1505, 285.0390, 255.0288, 227.0340, 187.0391 |
| 171 | 599.1030 | –2.1 | 10.66 | 216.26 | 212.92 | –1.55 | $C_{28}H_{24}O_{15}$ | $[M–H]^–$ | kaempferol-3-*O*-glucoside-6″-gallate or its isomer | PRR | FL | 483.1865, 465.2345, 213.0189, 151.0025 |
| 172 | 411.1626 | 0.1 | 10.72 | | 189.16 | | $C_{18}H_{28}O_9$ | $[M+Na]^+$ | isomer of chuanxiongoside A | CR | PL | 411.1623, 379.1248, 298.0547, 254.0284, |

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| | | | | | | | | | | | | 181.0120 |
| 173 | 353.0871 | –2.0 | 10.85 | 207.78 | 209.99 | 1.06 | $C_{16}H_{18}O_9$ | $[M–H]^-$ | isomer of chlorogenic acid | CR | OA | 191.0544 |
| 174 | 317.0644 | –3.7 | 11.20 | 162.67 | 163.29 | 0.39 | $C_{16}H_{12}O_7$ | $[M+H]^+$ | isomer of isorhamnetin | CF | FL | 302.0409, 274.0464, 107.0479 |
| 175 | 449.1075 | –0.7 | 11.27 | 199.51 | 199.67 | 0.08 | $C_{21}H_{20}O_{11}$ | $[M+H]^+$ | scutellarein or its isomer | SMRR | FL | 303.0459, 287.0537, 153.0174 |
| 176 | 331.1180 | –2.1 | 11.28 | 178.55 | 177.96 | –0.33 | $C_{18}H_{20}O_6$ | $[M–H]^-$ | tanshinol D or its isomer | SMRR | PQ | 331.118 |
| 177 | 463.0885 | 0.7 | 11.28 | 204.48 | 204.76 | 0.14 | $C_{21}H_{20}O_{12}$ | $[M–H]^-$ | isomer of quercetin-3-*O*-*β*-D-glucoside | CF | FL | 301.0309, 269.0449, 250.0625, 213.0557, 137.0229 |
| 178 | 613.1925 | –0.3 | 11.40 | 233.18 | 231.87 | –0.56 | $C_{31}H_{34}O_{13}$ | $[M–H]^-$ | mudanpioside A or its isomer | PRR | TP | 489.1033, 449.1069, 339.0856, 295.0593, 190.9980 |
| 179 | 447.0924 | –2.0 | 11.61 | 206.57 | 207.42 | 0.41 | $C_{21}H_{20}O_{11}$ | $[M–H]^-$ | isomer of luteolin-7-*O*-*β*-D-glucopyranoside | CF | FL | 327.1072, 285.0390, 284.0310, 121.0289 |
| 180 | 207.1002 | –6.6 | 11.68 | 144.09 | 143.68 | –0.29 | $C_{12}H_{14}O_3$ | $[M+H]^+$ | isomer of senkyunolide F | ASR | PL | 206.0822, 161.0948, 133.0634 |
| 181 | 419.1668 | –2.1 | 11.69 | | 196.22 | | $C_{20}H_{28}O_8$ | $[M+Na]^+$ | lobetyolin or its isomer | SMRR | OT | 403.1933, 279.0326, 225.0193, 191.0357 |
| 182 | 271.0589 | –4.3 | 11.83 | 155.02 | 153.70 | –0.85 | $C_{15}H_{10}O_5$ | $[M+H]^+$ | isomer of apigenin | SMRR | FL | 227.0329, 201.0501, 155.0474 |
| 183* | 477.1036 | –0.5 | 11.87 | 205.00 | 205.86 | 0.42 | $C_{22}H_{22}O_{12}$ | $[M–H]^-$ | isohamnetin-3-*O*-*β*-D-glucoside | PRR | FL | 301.0322, 271.0236 |
| 184 | 287.0557 | –1.4 | 11.88 | 160.47 | 161.04 | 0.35 | $C_{15}H_{12}O_6$ | $[M–H]^-$ | dihydrokaempferol or its isomer | PRR | FL | 271.0236, 269.0440 |
| 185 | 593.1517 | 0.9 | 11.95 | 236.89 | 238.96 | 0.87 | $C_{27}H_{30}O_{15}$ | $[M–H]^-$ | isomer of safflor yellow A | CF | FL | 335.0558, 325.0710 |
| 186 | 433.1436 | –7.6 | 12.10 | | 201.52 | | $C_{20}H_{26}O_9$ | $[M+Na]^+$ | 3-*O*-caffeoylquinic acid butyl ester or its isomer | SMRR | OA | 386.7082, 263.0718, 115.0524 |
| 187 | 647.1617 | –0.1 | 12.27 | 247.60 | 247.95 | 0.14 | $C_{30}H_{32}O_{16}$ | $[M–H]^-$ | isomer of galloyloxypaeoniflorin | PRR | TP | 643.1665, 464.1003, 277.0517 |
| 188 | 359.1824 | –8.1 | 12.37 | 132.91 | 152.39 | –0.28 | $C_{21}H_{26}O_5$ | $[M+H]^+$ | isomer of 14-acetoxy-12-senecioyloxytetradeca-2E,8E,10E-trien- 4,6-diyn-1-ol | ASR | OT | 359.1814, 337.1685, 196.0846, 191.0330, 151.0730 |
| 189 | 574.1563 | –0.5 | 12.37 | 237.43 | 238.97 | 0.65 | $C_{27}H_{29}NO_{13}$ | $[M–H]^-$ | isomer of isocartormin | CF | AL | 519.0911, 465.2695, 424.1030, 364.0816, 244.0255 |
| 190 | 359.0767 | -1.4 | 12.58 | | 241.81 | | $C_{18}H_{16}O_8$ | $[M–H]^-$ | rosmarinic acid | SMRR | OA | 197.0448, 179.0341 |

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| 191 | 197.0797 | –5.9 | 12.70 | 210.16 | 210.40 | 0.12 | $C_{10}H_{12}O_4$ | $[M+H]^+$ | isomer of paeonilactone B | PRR | TP | 161.0584, 133.0632, 105.0318 |
| 192 | 479.1557 | –0.3 | 12.71 | 292.07 | 292.30 | 0.08 | $C_{23}H_{28}O_{11}$ | $[M–H]^–$ | paeonins B or its isomer | PRR | TP | 311.0917, 245.0813 |
| 193 | 121.0292 | –2.7 | 12.81 | 220.27 | 223.58 | 1.50 | $C_7H_6O_2$ | $[M–H]^–$ | isomer of benzoic acid | PRR | OA | 77.0392 |
| 194 | 225.1105 | –7.4 | 12.90 | 159.95 | 159.88 | –0.05 | $C_{12}H_{16}O_4$ | $[M+H]^+$ | senkyunolide I or its isomer | CR | PL | 207.1003, 189.0901, 128.0604, 105.0689 |
| 195 | 189.0899 | –6.0 | 12.92 | 138.92 | 140.19 | 0.92 | $C_{12}H_{12}O_2$ | $[M+H]^+$ | isomer of (Z)-3-butylidenephthalide | ASR/CR | PL | 145.0163, 115.0530, 105.0688, 91.0523, 77.0365 |
| 196 | 207.1017 | 0.5 | 12.94 | 143.44 | 144.79 | 0.94 | $C_{12}H_{14}O_3$ | $[M+H]^+$ | senkyunolide F or its isomer | CR | PL | 189.0908, 161.0953 |
| 197 | 165.0894 | –9.7 | 12.95 | 146.31 | 147.32 | 0.69 | $C_{10}H_{12}O_2$ | $[M+H]^+$ | isomer of eugenol | CR | OT | 160.9889, 145.0163, 133.0637, 115.0530, 91.0523 |
| 198 | 574.1542 | –4.2 | 12.99 | 231.90 | 234.38 | 1.07 | $C_{27}H_{29}NO_{13}$ | $[M–H]^–$ | isomer of isocartormin | CF | AL | 547.1542, 527.2531 |
| 199 | 389.1806 | 0.0 | 13.17 | | 138.47 | | $C_{18}H_{28}O_9$ | $[M+H]^+$ | isomer of chuanxiongoside A | CR | PL | 381.1939, 359.1782, 277.0953, 233.0683, 189.0419 |
| 200 | 383.1340 | –1.9 | 13.18 | 193.89 | 194.78 | 0.46 | $C_{18}H_{24}O_9$ | $[M–H]^–$ | (-)-4-hydroxybenzoic-4-*O*-[6'-*O*-(2-methylbutyryl)-*β*-D-glucopyranoside] or its isomer | CF | OT | 273.0743, 167.0344 |
| 201 * | 493.1131 | –1.9 | 13.38 | 207.08 | 208.13 | 0.50 | $C_{26}H_{22}O_{10}$ | $[M–H]^–$ | salvianolic acid A | SMRR | OA | 295.0604, 185.0233 |
| 202 | 289.0694 | –4.4 | 13.83 | 160.65 | 160.90 | 0.16 | $C_{15}H_{12}O_6$ | $[M+H]^+$ | isomer of (-)-eriodictyol | CF | OT | 169.0117, 147.0429, 119.0478 |
| 203 | 613.1556 | 0.0 | 13.86 | 241.30 | 241.18 | –0.05 | $C_{30}H_{30}O_{14}$ | $[M–H]^–$ | isosafflomin C or its isomer | CF | FL | 551.1553, 361.1073, 241.0495, 119.0494 |
| 204 | 179.0710 | –2.3 | 13.87 | 148.21 | 147.27 | –0.63 | $C_{10}H_{12}O_3$ | $[M–H]^–$ | 4-hydroxy-3-methoxypropiophenone or its isomer | CR | PL | 109.0284 |
| 205 | 221.0794 | –6.4 | 13.93 | 142.28 | 142.29 | 0.01 | $C_{12}H_{12}O_4$ | $[M+H]^+$ | isomer of senkyunolide D | CR | PL | 165.0169, 161.0220, 128.0605, 105.0318 |
| 206 | 179.1057 | –5.4 | 14.05 | 140.06 | 141.42 | 0.97 | $C_{11}H_{14}O_2$ | $[M+H]^+$ | isomer of methyl eugenol | CR | PP | 133.0637, 115.0525, 103.0526, 91.0522, 77.0367 |
| 207 | 207.1002 | –6.8 | 14.07 | 143.85 | 145.11 | 0.88 | $C_{12}H_{14}O_3$ | $[M+H]^+$ | isomer of senkyunolide F | ASR/CR | PL | 207.1009, 189.0453 |

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| 208 | 189.0899 | –5.8 | 14.07 | 140.38 | 142.98 | 1.85 | $C_{12}H_{12}O_2$ | $[M+H]^+$ | isomer of (*Z*)-3-butylidenephthalide | ASR | PL | 133.0637, 115.0525, 105.0689, 91.0522, 77.0367 |
| 209 | 503.2131 | –0.5 | 14.11 | 219.83 | 219.91 | –0.04 | $C_{23}H_{36}O_{12}$ | $[M–H]^–$ | isomer of ligusticoside B | CR | PL | 499.1206, 313.9866, 237.0758 |
| 210 | 273.0741 | –6.1 | 14.23 | 159.16 | 159.38 | 0.14 | $C_{15}H_{12}O_5$ | $[M+H]^+$ | isomer of naringenin | PRR | FL | 182.1527 |
| 211 | 645.1806 | –3.0 | 14.48 | 247.53 | 245.28 | –0.91 | $C_{31}H_{34}O_{15}$ | $[M–H]^–$ | 6-*O*-vanillyoxypaeoniflorin or its isomer | PRR | TP | 639.1348, 543.2808, 477.1962, 301.0339, 267.0293 |
| 212 | 631.1657 | –1.8 | 14.76 | 224.33 | 225.06 | 0.32 | $C_{30}H_{32}O_{15}$ | $[M–H]^–$ | isomer of galloylpaeoniflorin | PRR | TP | 631.1657, 563.3044, 399.0902, 313.0551, 169.0133 |
| 213 | 531.1511 | 0.6 | 15.08 | 230.59 | 230.20 | –0.17 | $C_{26}H_{28}O_{12}$ | $[M–H]^–$ | isomer of chuanxiongoside D | CR | PP | 509.2170, 191.0554 |
| 214 | 941.3087 | 0.3 | 15.13 | 292.60 | 294.86 | 0.77 | $C_{46}H_{54}O_{21}$ | $[M–H]^–$ | isomer of paeonidanin E | PRR | TP | 923.2977, 893.2860, 679.2224, 327.1082, 121.0287 |
| 215* | 537.1039 | 0.1 | 15.33 | 242.50 | 242.66 | 0.07 | $C_{27}H_{22}O_{12}$ | $[M–H]^–$ | lithospermic acid | SMRR | OA | 519.0926, 321.0393, 295.0600, 185.0236, 105.0287 |
| 216* | 717.1454 | –0.9 | 15.34 | 246.06 | 245.13 | –0.38 | $C_{36}H_{30}O_{16}$ | $[M–H]^–$ | salvianolic acid B | SMRR | OA | 519.0926, 339.0500, 321.0393, 295.0600 |
| 217 | 243.1217 | –4.2 | 15.55 | | 192.08 | | $C_{12}H_{18}O_5$ | $[M+H]^+$ | isomer of 3-hydroxy-4,5,6,7-tetrahydro-6,7-dihydroxy -3-butylphthalide | CR | PL | 205.0142, 177.1112, 155.0696, 99.0423 |
| 218 | 615.1718 | –0.2 | 15.63 | 232.89 | 234.04 | 0.49 | $C_{30}H_{32}O_{14}$ | $[M–H]^–$ | mudanpioside H or its isomer | PRR | TP | 615.1698, 571.2394, 485.1646, 315.0494 |
| 219* | 599.1762 | –1.3 | 15.73 | 223.15 | 221.57 | –0.71 | $C_{30}H_{32}O_{13}$ | $[M–H]^–$ | benzoyloxypaeoniflorin | PRR | TP | 477.1405, 281.0657, 137.0237 |
| 220 | 413.0868 | –2.3 | 16.04 | 192.92 | 192.46 | –0.24 | $C_{21}H_{18}O_9$ | $[M–H]^–$ | isomer of saffloflavonesides A | CF | FL | 311.0911, 283.0974 |
| 221 | 475.3061 | –0.9 | 16.17 | 223.29 | 227.29 | 1.79 | $C_{28}H_{44}O_6$ | $[M–H]^–$ | 3*β*,4*β*,23,29-tetrahy-droxy-24-norolean-12-en-28-oic acid or its isomer | PRR | TP | 442.1276, 429.2923, 407.0954, 405.0762 |
| 222 | 629.1869 | –1.1 | 16.20 | 227.44 | 224.94 | –1.1 | $C_{31}H_{34}O_{14}$ | $[M–H]^–$ | isomer of mudanpioside B | PRR | TP | 477.1408, 461.1443, 459.1293311.0760, 167.0342 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 223 | 1087.2570 | –0.1 | 16.67 | 315.86 | 317.97 | 0.67 | $C_{49}H_{52}O_{28}$ | $[M–H]^-$ | isomer of carthorquinoside A | CF | FL | 625.1399, 461.1077, 449.1007, 271.0602 |
| 224 | 465.1770 | 0.8 | 17.28 | 211.82 | 210.70 | –0.53 | $C_{23}H_{30}O_{10}$ | $[M–H]^-$ | paeoniflorol or its isomer | PRR | TP | 447.2226, 329.1746, 289.0704, 165.0550 |
| 225 | 309.0863 | –2.1 | 17.29 | | 164.87 | | $C_{17}H_{12}N_2O_4$ | $[M+H]^+$ | flazine or its isomer | ASR | AL | 263.0813, 233.0687, 207.0143, 158.9725 |
| 226 | 599.1764 | –1.1 | 17.32 | 222.99 | 223.98 | 0.45 | $C_{30}H_{32}O_{13}$ | $[M–H]^-$ | isomer of benzoyloxypaeoniflorin | PRR | TP | 477.1491, 137.0236 |
| 227 * | 301.0343 | –3.6 | 17.33 | | 159.20 | | $C_{15}H_{10}O_7$ | $[M–H]^-$ | quercetin | CF | FL | 285.0394 |
| 228 | 717.1438 | –3.2 | 17.36 | 239.40 | 240.58 | 0.49 | $C_{36}H_{30}O_{16}$ | $[M–H]^-$ | isomer of salvianolic acid B | SMRR | OA | 339.0510, 321.0392, 295.0607 |
| 229 | 225.0766 | –0.9 | 17.41 | 149.29 | 147.89 | –0.94 | $C_{11}H_{14}O_5$ | $[M–H]^-$ | butyl gallate or its isomer | PRR | OT | 188.0061 |
| 230 | 955.2207 | 5.9 | 17.43 | 301.97 | 298.55 | –1.13 | $C_{44}H_{44}O_{24}$ | $[M–H]^-$ | precarthamin or its isomer | CF | FL | 861.2836, 489.2705, 451.1035, 289.0708, 125.0237 |
| 231 | 745.2325 | –3.3 | 17.43 | 262.21 | 261.03 | –0.45 | $C_{36}H_{42}O_{17}$ | $[M–H]^-$ | paeoniflorin B or its isomer | PRR | TP | 635.1617, 521.2748, 327.0488, 297.0398, 177.0914 |
| 232 | 331.0440 | –2.6 | 17.45 | 161.88 | 163.35 | 0.90 | $C_{16}H_{10}O_8$ | $[M+H]^+$ | 3,4‘-*O*-dimethylellagic acid or its isomer | PRR | OA | 299.0188, 233.0685, 189.0429, 138.0316 |
| 233 | 445.2074 | –1.2 | 17.45 | 213.16 | 215.87 | 1.27 | $C_{21}H_{34}O_{10}$ | $[M–H]^-$ | isomer of (Z)-(1*S*,5*R*)-*β*-pinen-10-yl-*β*-vicianoside | PRR | TP | 359.2205, 329.2323, 201.1129 |
| 234 * | 731.1623 | 0.8 | 17.47 | | 253.90 | | $C_{37}H_{32}O_{16}$ | $[M–H]^-$ | 9-methyl lithospermate B | SMRR | OA | 341.1058, 295.0605 |
| 235 * | 491.0972 | –2.4 | 17.58 | | 201.20 | | $C_{26}H_{20}O_{10}$ | $[M–H]^-$ | salvianolic acid C | SMRR | OA | 311.0547, 293.0440, 249.0549, 179.0338, 135.0440 |
| 236 | 584.2758 | 0.5 | 17.60 | 237.35 | 234.32 | –1.28 | $C_{34}H_{37}N_3O_6$ | $[M+H]^+$ | safflospermidine B or its isomer | CF | AL | 438.2381, 420.2282, 275.1743, 147.0428 |
| 237 | 207.1004 | –5.9 | 17.63 | 144.39 | 144.44 | 0.04 | $C_{12}H_{14}O_3$ | $[M+H]^+$ | isomer of 4-hydroxy-3-butylphthalide | CR | PL | 207.0272, 205.1029, 198.0505, 186.0935 |
| 238 | 909.2109 | 1.5 | 17.64 | 317.82 | 313.63 | –1.32 | $C_{43}H_{42}O_{22}$ | $[M–H]^-$ | carthamin or its isomer | CF | FL | 581.1852, 537.1394, 339.0859, 293.0439, 135.0440 |
| 239 | 355.1177 | –2.8 | 17.68 | 184.72 | 183.88 | –0.45 | $C_{20}H_{20}O_6$ | $[M–H]^-$ | isomer of coniferyl ferulate | ASR | OT | 343.2137, 297.9741, 259.1688 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 240 | 205.0857 | –1.3 | 17.70 | 140.18 | 138.41 | –1.27 | $C_{12}H_{12}O_3$ | $[M+H]^+$ | isomer of 3-Butylidene-7-hydroxyphthalide | ASR | PL | 198.0505, 168.0559, 151.0531, 141.0687 |
| 241 | 189.0897 | –6.7 | 17.70 | 133.55 | 132.70 | –0.64 | $C_{12}H_{12}O_2$ | $[M+H]^+$ | isomer of (*Z*)-3-butylidenephthalide | ASR | PL | 168.0559, 141.0687, 128.0605, 91.0523 |
| 242 | 271.0601 | –4.0 | 17.74 | 271.44 | 271.22 | –0.08 | $C_{15}H_{12}O_5$ | $[M–H]^–$ | isomer of naringenin | PRR | FL | 234.0661, 177.0909, 147.0799, 109.0285 |
| 243 * | 583.1815 | –1.0 | 17.74 | 236.84 | 235.96 | –0.37 | $C_{30}H_{32}O_{12}$ | $[M–H]^–$ | benzoylpaeoniflorin | PRR | TP | 553.1706, 431.1366, 295.0603, 165.0547, 121.0285 |
| 244 | 629.1867 | –1.4 | 17.74 | 326.75 | 329.68 | 0.89 | $C_{31}H_{34}O_{14}$ | $[M–H]^–$ | mudanpioside B or its isomer | PRR | TP | 553.1706, 431.1366, 165.0547, 121.0285 |
| 245 | 427.1382 | 4.0 | 17.74 | | 197.05 | | $C_{18}H_{28}O_9$ | $[M+K]^+$ | chuanxiongoside A or its isomer | CR | PL | 309.0804, 263.0001, 161.0586, 105.0317, 77.0368 |
| 246 | 585.1978 | 1.9 | 17.77 | 231.58 | 231.70 | 0.06 | $C_{30}H_{32}O_{12}$ | $[M+H]^+$ | isomer of 2'-*O*-benzoylpaeoniflorin | PRR | TP | 443.0448, 309.2784, 179.0832, 105.0317 |
| 247 | 197.0794 | –7.3 | 17.77 | 235.64 | 237.19 | 0.66 | $C_{10}H_{12}O_4$ | $[M+H]^+$ | isomer of paeonilactone B | PRR | TP | 181.0647, 161.0952, 105.0317, 77.0368 |
| 248 * | 269.0445 | –3.8 | 17.78 | 153.34 | 154.55 | 0.79 | $C_{15}H_{10}O_5$ | $[M–H]^–$ | apigenin | CF | FL | 255.2369, 252.0398, 195.0430, 119.0495 |
| 249 | 277.1421 | –4.7 | 17.80 | 163.73 | 165.41 | 1.03 | $C_{16}H_{20}O_4$ | $[M+H]^+$ | dibutylphthalate or its isomer | CR | PL | 249.1475, 207.1004, 115.0531, 91.0526 |
| 250 | 361.1639 | –1.9 | 17.83 | 189.74 | 191.15 | 0.74 | $C_{20}H_{24}O_6$ | $[M+H]^+$ | lariciresinol or its isomer | SMRR | OT | 305.0314, 283.0613, 222.0870, 123.0789 |
| 251 * | 285.0392 | –4.3 | 17.83 | | 157.78 | | $C_{15}H_{10}O_6$ | $[M–H]^–$ | kaempferol | CF | FL | 269.045 |
| 252 | 357.1696 | –3.3 | 17.84 | 195.33 | 194.52 | –0.41 | $C_{21}H_{26}O_5$ | $[M–H]^–$ | isomer of 14-acetoxy-12-senecioyloxytetradeca-2E,8E,10E-trien- 4,6-diyn-1-ol | CR/ASR | OT | 349.2409, 295.0605, 269.0441, 253.0480, 161.0592 |
| 253 | 217.0480 | –6.9 | 17.86 | 135.22 | 134.35 | –0.65 | $C_{12}H_8O_4$ | $[M+H]^+$ | methoxsalen or its isomer | CR | PP | 174.0300, 167.0819, 130.0648 |
| 254 | 297.1109 | –7.8 | 17.88 | 182.92 | 184.46 | 0.84 | $C_{18}H_{18}O_4$ | $[M–H]^–$ | tanshinol C or its isomer | SMRR | PQ | 291.1958, 275.2000, 271.0242, 211.0386, 165.1275 |
| 255 | 281.0811 | –3.0 | 17.92 | 160.30 | 160.20 | –0.07 | $C_{17}H_{14}O_4$ | $[M–H]^–$ | dihydronortanshinone or its isomer | SMRR | TP | 271.0242, 247.1329, 243.0276, 241.0901 |
| 256 | 183.1382 | –4.8 | 17.93 | 152.28 | 151.44 | –0.55 | $C_{11}H_{20}O_2$ | $[M–H]^–$ | 4-pentylcyclohex-3-ene-1$\alpha$,2$\beta$-diol or its isomer | CR | OT | 183.1382, 177.0910 |
| 257 | 489.3567 | –1.5 | 17.96 | 228.20 | 228.84 | 0.28 | $C_{30}H_{48}O_5$ | $[M+H]^+$ | chuanxiongins D or its isomer | CR | PL | 393.1375, 349.1450, 263.0699, 147.0429 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 258 | 355.1181 | –1.6 | 18.00 | 191.55 | 190.67 | –0.46 | $C_{20}H_{20}O_6$ | $[M–H]^-$ | coniferyl ferulate or its isomer | CR | OT | 329.2325, 211.1327, 171.1016, 139.1123 |
| 259 | 585.1981 | 2.6 | 18.01 | 229.65 | 230.90 | 0.54 | $C_{30}H_{32}O_{12}$ | $[M+H]^+$ | isomer of 2′-*O*-benzoylpaeoniflorin | PRR | TP | 537.2741, 393.1375, 325.1446, 227.0359, 211.0661 |
| 260 | 297.1475 | –3.3 | 18.02 | | 168.00 | | $C_{19}H_{20}O_3$ | $[M+H]^+$ | isocryptotanshinone II or its isomer | SMRR | PQ | 269.1532, 251.1419, 237.0909, 209.0952, 181.0998, 141.0681 |
| 261 | 205.0861 | –4.3 | 18.09 | 146.89 | 145.11 | –1.21 | $C_{12}H_{14}O_3$ | $[M–H]^-$ | 3-butyl-4-hydroxy-2-benzofuran-1(3H)-one or its isomer | ASR | OT | 205.0861, 179.0705 |
| 262 | 179.0705 | –4.8 | 18.10 | 146.89 | 147.34 | 0.30 | $C_{10}H_{12}O_3$ | $[M–H]^-$ | coniferyl alcohol or its isomer | CR | OT | 179.0705, 162.1007 |
| 263 | 341.1371 | –3.7 | 18.13 | 174.26 | 174.06 | –0.11 | $C_{20}H_{20}O_5$ | $[M+H]^+$ | isomer of chuanxiongnolide L3 | CR | PL | 247.0644, 237.0823, 191.1055, 120.9725 |
| 264 | 285.1490 | –2.1 | 18.14 | 181.67 | 183.74 | 1.14 | $C_{18}H_{22}O_3$ | $[M–H]^-$ | cryptoacetalide or its isomer | SMRR | TP | 225.1378, 199.1325, 185.1175, 163.0403 |
| 265 | 343.0451 | –2.4 | 18.17 | 170.32 | 171.44 | 0.66 | $C_{17}H_{12}O_8$ | $[M–H]^-$ | 3,3′,4-*O*-trimethyl ellagic acid or its isomer | PRR | OA | 312.9978, 297.9748, 269.9799, 225.0920 |
| 266 | 209.1175 | –3.9 | 18.20 | 150.71 | 150.72 | 0.01 | $C_{12}H_{18}O_3$ | $[M–H]^-$ | sedanonic acid or its isomer | CR | OA | 209.1175, 197.1176, 165.1288 |
| 267 | 223.1331 | –3.8 | 18.21 | 153.71 | 154.80 | 0.71 | $C_{13}H_{20}O_3$ | $[M–H]^-$ | blumenol A or its isomer | CF | OT | 223.1331, 209.1175, 165.1288 |
| 268 | 311.1275 | –0.9 | 18.21 | | 170.60 | | $C_{19}H_{18}O_4$ | $[M+H]^+$ | tanshinone IIB or its isomer | SMRR | PQ | 293.2103, 267.1358, 252.1134, 237.0823 |
| 269 | 355.1176 | –3.0 | 18.28 | 181.59 | 181.86 | 0.15 | $C_{20}H_{20}O_6$ | $[M–H]^-$ | isomer of coniferyl ferulate | CR/ASR | OT | 269.0434, 257.1538, 247.1330, 185.1127, 162.8383 |
| 270 | 205.0851 | –4.0 | 18.29 | 165.20 | 166.59 | 0.84 | $C_{12}H_{12}O_3$ | $[M+H]^+$ | senkyunolide E or its isomer | CR | PL | 165.0171 |
| 271 | 207.1006 | –4.5 | 18.32 | 143.52 | 143.15 | –0.26 | $C_{12}H_{14}O_3$ | $[M+H]^+$ | isomer of 4-hydroxy-3-butylphthalide | CR | PL | 207.1006, 205.0851, 197.0945, 187.0378 |
| 272 | 205.0863 | –3.7 | 18.33 | 195.16 | 195.33 | 0.08 | $C_{12}H_{14}O_3$ | $[M–H]^-$ | isomer of Senkyunolide F | CR | PL | 162.8383, 160.8416 |
| 273 | 203.0705 | –4.4 | 18.51 | 145.14 | 143.67 | 1.03 | $C_{12}H_{12}O_3$ | $[M–H]^-$ | senkyunolide B or its isomer | CR | PL | 173.0234, 160.0163, 145.0297, 132.0211 |
| 274 | 413.1978 | 4.6 | 18.51 | | 194.71 | | $C_{24}H_{28}O_6$ | $[M+H]^+$ | isomer of chuanxiongnolide L4 | CR | PL | 333.1365, 273.0295, 267.1364, 247.0375, 229.6614 |
| 275 | 205.0839 | –10.0 | 18.53 | 139.94 | 140.05 | 0.08 | $C_{12}H_{12}O_3$ | $[M+H]^+$ | isomer of 3-butylidene-7-hydroxyphthalide | ASR | PL | 205.0839, 200.1059, 191.1056, 182.0949, |
| 276 | 259.1705 | 0.5 | 18.55 | 178.06 | 175.00 | –1.72 | $C_{17}H_{24}O_2$ | $[M–H]^-$ | falcarindiol or its isomer | CR | TP | 259.1705, 255.1384, 249.1856 |
| 277 | 279.1593 | 0.7 | 18.57 | 160.42 | 161.32 | 0.56 | $C_{16}H_{22}O_4$ | $[M+H]^+$ | senkyunolide M or its isomer | CR | PL | 233.1556, 191.1070 |
| 278 | 311.1268 | –3.1 | 18.65 | | 168.68 | | $C_{19}H_{18}O_4$ | $[M+H]^+$ | tanshinaldehyde or its isomer | SMRR | PQ | 265.1212, 223.0745, 179.0833, 165.0683 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 279 | 271.1695 | –3.3 | 18.77 | 181.01 | 181.80 | 0.44 | $C_{18}H_{24}O_2$ | $[M–H]^-$ | isomer of (+)-miltiorolide A | SMRR | OT | 271.1688, 241.1588, 227.1795 |
| 280 | 191.1054 | –6.6 | 18.84 | 137.95 | 137.39 | –0.41 | $C_{12}H_{14}O_2$ | $[M+H]^+$ | isomer of senkyunolide A | ASR | PL | 191.1048 |
| 281 | 313.1441 | –1.5 | 19.32 | | 184.37 | | $C_{19}H_{22}O_4$ | $[M–H]^-$ | neocryptotanshinone or its isomer | SMRR | PQ | 269.1537, 241.1587, 226.0994, 213.0914 |
| 282 | 397.2012 | –2.2 | 19.80 | 196.87 | 197.04 | 0.09 | $C_{24}H_{30}O_5$ | $[M–H]^-$ | chuanxiongnolide A or its isomer | CR | PL | 187.0757, 161.0958, 145.0282, |
| 283 | 381.2028 | –8.5 | 19.81 | 188.23 | 188.56 | 0.18 | $C_{24}H_{28}O_4$ | $[M+H]^+$ | angelicide or its isomer | ASR | PL | 307.1657, 251.1057, 191.1060, 178.0767, 165.0685 |
| 284 | 271.1695 | –3.3 | 20.06 | 177.73 | 179.64 | 1.07 | $C_{18}H_{24}O_2$ | $[M–H]^-$ | isomer of (+)-miltiorolide A | SMRR | OT | 271.1695 |
| 285 | 293.2109 | –4.5 | 20.08 | 178.64 | 178.80 | 0.09 | $C_{18}H_{30}O_3$ | $[M–H]^-$ | isomer of 2,3-*trans*-4,5-*cis*-diene-6-carbonyl stearic acid | SMRR | OT | 231.1741 |
| 286* | 277.0947 | –3.2 | 20.93 | 151.64 | 156.83 | 0.98 | $C_{18}H_{12}O_3$ | $[M+H]^+$ | Tanshinone I | SMRR | PQ | 249.0902, 221.0956, 178.0762, 141.0686 |
| 287 | 397.1676 | 4.8 | 21.24 | 194.67 | 194.90 | 0.12 | $C_{23}H_{26}O_6$ | $[M–H]^-$ | salmiltiorin D or its isomer | SMRR | TP | 397.1676, 389.1396, 365.2293 |
| 288 | 293.2119 | –1.0 | 21.45 | 179.56 | 180.91 | 0.76 | $C_{18}H_{30}O_3$ | $[M–H]^-$ | isomer of 2,3-*trans*-4,5-*cis*-diene-6-carbonyl stearic acid | SMRR | OT | 231.1744 |
| 289 | 881.7605 | 1.4 | 22.40 | | 222.38 | | $C_{57}H_{100}O_6$ | $[M+H]^+$ | 1,3-linolein-2-olein or its isomer | SMRR | OT | 721.4363, 525.2888, 427.1467, 293.0674, 252.0444 |
| 290 | 795.1740 | –0.3 | 22.80 | | 237.82 | | $C_{36}H_{36}O_{19}$ | $[M+Na]^+$ | luteolin-7-*O*-D-gentibioside or its isomer | SMRR | FL | 513.1987, 333.0966, 311.2848, 205.0146 |
| 291 | 279.2333 | 1.2 | 24.36 | 179.25 | 178.40 | –0.48 | $C_{18}H_{32}O_2$ | $[M–H]^-$ | isomer of linoleic acid | CR | OA | 279.2333 |
| 292 | 255.2324 | –2.2 | 25.05 | 174.27 | 174.12 | –0.08 | $C_{16}H_{32}O_2$ | $[M–H]^-$ | palmitic scid or its isomer | ASR | OA | 255.2324 |
| 293 | 399.3650 | 7.2 | 25.64 | 224.10 | 224.86 | 0.34 | $C_{28}H_{46}O$ | $[M+H]^+$ | isomer of Δ7-stigmasta-7-ene-3-one | SMRR | OT | 377.1246, 333.0985, 288.0652, 245.0456 |
| 294 | 371.0971 | –0.4 | 25.87 | | 176.54 | | $C_{16}H_{18}O_{10}$ | $[M+H]^+$ | isomer of isofraxoside | CR | PP | 251.9671 |

***:** The components confirmed by comparison with the reference standards.

FL: Flavonoid, TP: Terpenoid, PQ: Phenanthrenequinone, AL: Alkaloids, OA: Organic acid, PL: Phthalide, PP: Phenylpropanoid, OT: Others

CF: Carthami Flos, PRR: Paeoniae Radix Rubra, CR: Chuanxiong Rhizoma, SMRR: Salviae Miltiorrhizae Radix et Rhizoma, ASR: Angelicae Sinensis Radix.