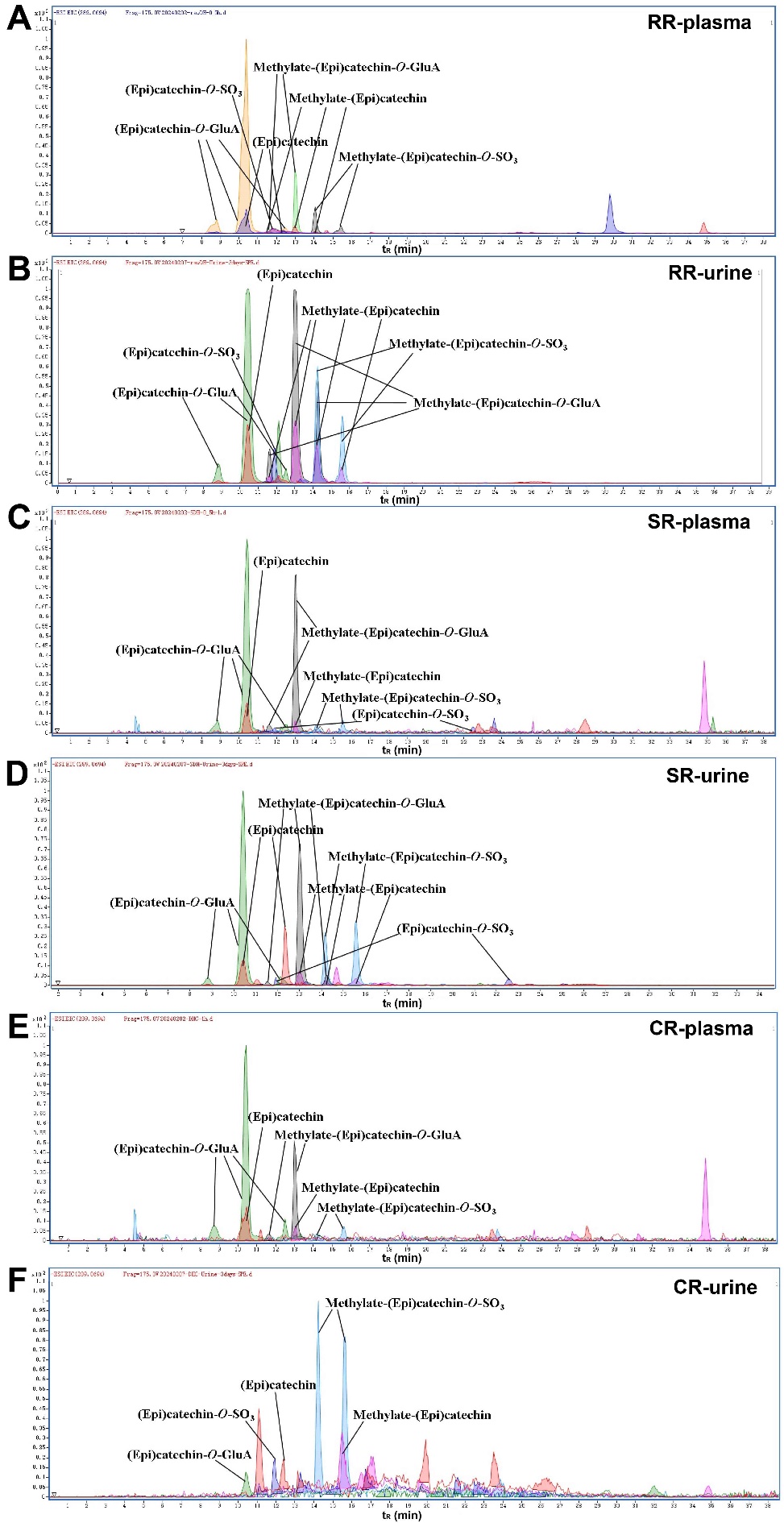
Supplementary Material

# Supplementary Figures and Tables

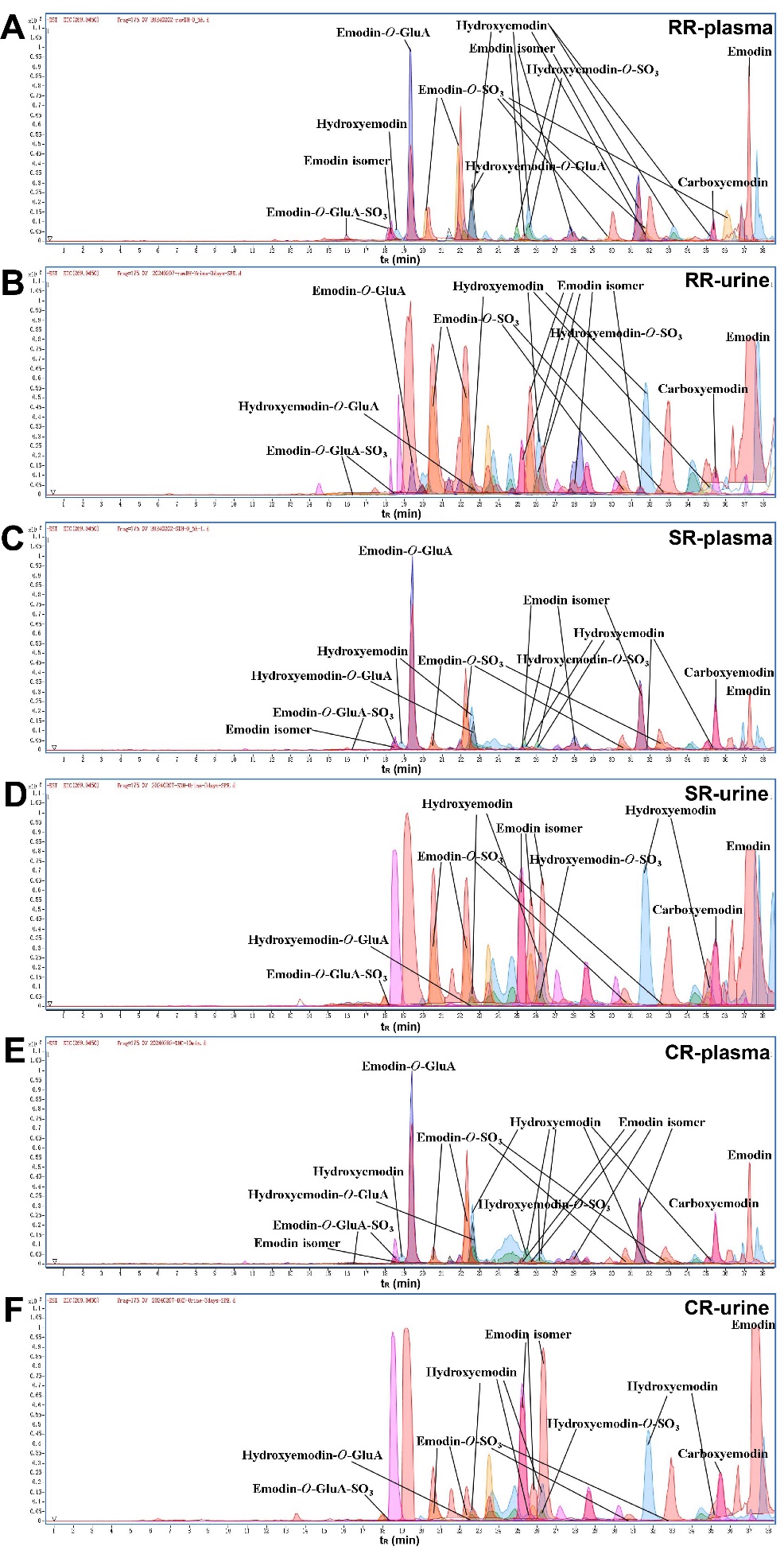
## Supplementary Figures



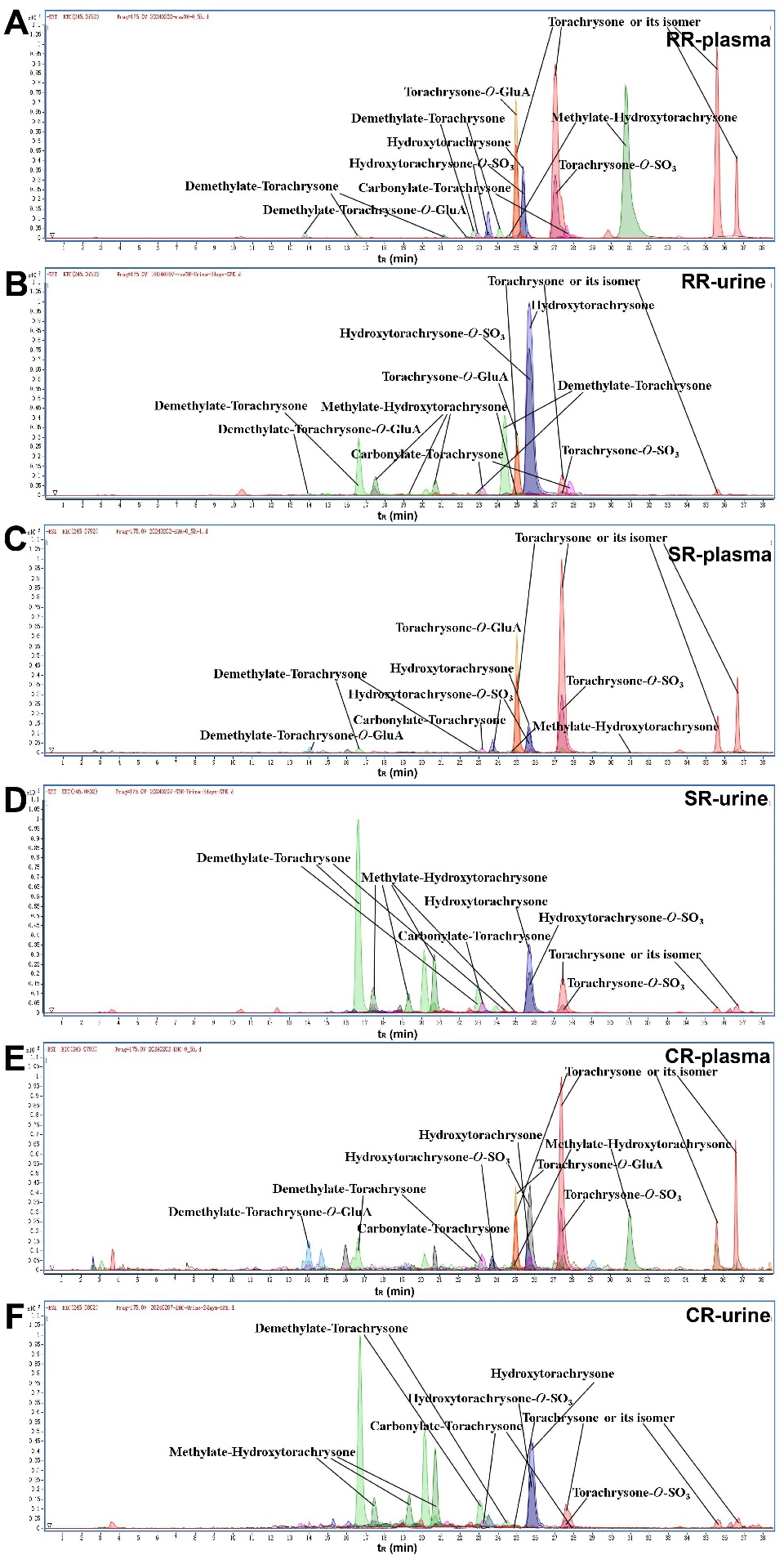
**Supplementary Figure 1.** The total ion chromatograms (TICs) of RR (A), SR (B) and CR (C) samples and their three fractions determined by UPLC-Q-TOF-MS in negative ion mode.



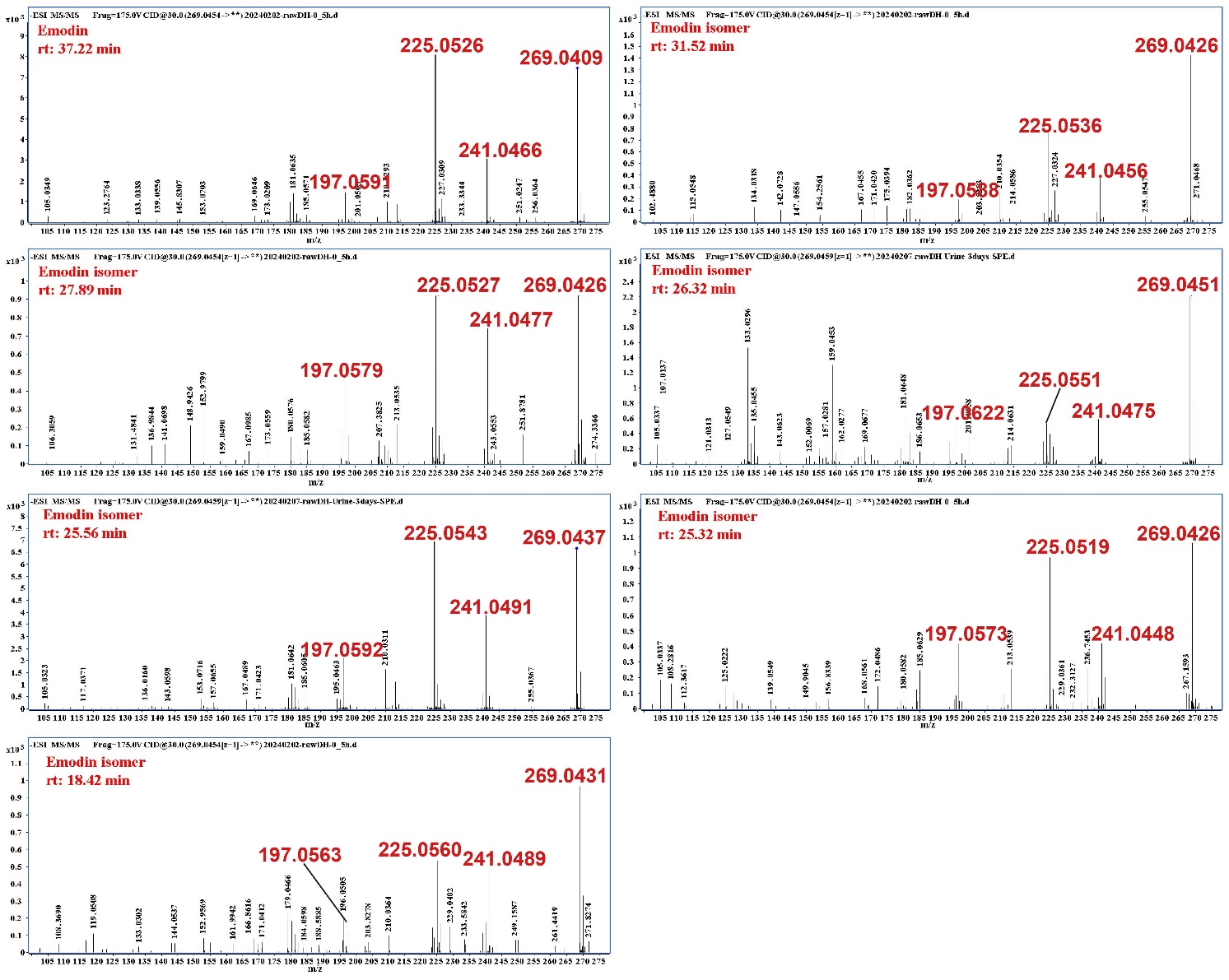
**Supplementary Figure 2.** The EICs of (epi)catechin and its metabolites in rats.



**Supplementary Figure 3.** The EICs of emodin and its metabolites in rats.



**Supplementary Figure 4.** The EICs of torachrysone and its metabolites in rats.



**Supplementary Figure 5.** The MS/MS spectra of emodin and its isomers.



**Supplementary Figure 4.** Peak area comparison of (A) torachrysone and (B) emodin anthrone in three processed products of rhubarb.

## Supplementary Tables

**Supplementary Table 1** The identification results of compounds in RR, SR and CR.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Num. | Name | Rt  (min) | *m/z*  (Neg) | Formula | MS/MS | RR | SR | CR | Sample |
| C1 | Ornithine | 2.84 | 131.0834 | C5H12N2O2 | 114.0550 | ＋ | ＋ | ＋ | Fr1 |
| C2 | Arginine | 2.84 | 173.1045 | C6H14N4O2 | 131.0838 | ＋ | ＋ | ＋ | Zong |
| C3 | Glutamine | 2.89 | 145.0621 | C5H10N2O3 | 127.0520, 109.0412 | ＋ | ＋ | ＋ | Zong |
| C4 | Histidine | 2.89 | 154.0621 | C6H9N3O2 | 137.0350, 110.0727 | ＋ | ＋ | - | Zong |
| C5 | *N*2-Fructopyranosylarginine | 2.89 | 335.1555 | C12H24N4O7 | 173.1031, 131.0830 | ＋ | ＋ | ＋ | Zong |
| C6 | Sucrose | 3.13 | 341.1139 | C12H22O11 | 179.0553, 161.0448, 101.0245 | ＋ | - | ＋ | Zong |
| C7 | Raffinose | 3.30 | 503.1625 | C18H32O16 | 323.0952, 179.0551 | ＋ | - | ＋ | Zong |
| C8 | Malic acid | 3.70 | 133.0137 | C4H6O5 | 115.0037 | ＋ | ＋ | ＋ | Zong |
| C9 | 2/6/1'/4'/6'-*O*-Galloylsucrose | 3.82 | 493.1188 | C19H26O15 | 331.0649, 169.0131, 125.0237 | ＋ | ＋ | ＋ | Zong |
| C10 | Galloylglucose | 3.99 | 331.0651 | C13H16O10 | 211.0243, 169.0139, 151.0036, 125.0244 | ＋ | ＋ | ＋ | Zong |
| C11 | Citramalic acid or its isomer | 4.52 | 147.0295 | C5H8O5 | 129.0189, 103.0405 | ＋ | ＋ | ＋ | Zong |
| C12 | Citric acid | 4.52 | 191.0191 | C6H8O7 | 111.0095 | ＋ | ＋ | ＋ | Zong |
| C13 | Galloylglucose | 4.87 | 331.0668 | C13H16O10 | 211.0238, 169.0129, 151.0033, 125.0237 | ＋ | ＋ | ＋ | Zong |
| C14 | 2/6/1'/4'/6'-*O*-Galloylsucrose | 5.16 | 493.1183 | C19H26O15 | 331.0660, 169.0124, 125.0242 | ＋ | ＋ | ＋ | Zong |
| C15 | Tyrosine | 5.16 | 180.0662 | C9H11NO3 | 163.0392, 119.0503 | ＋ | ＋ | ＋ | Zong |
| C16 | Citramalic acid or its isomer | 5.33 | 147.0296 | C5H8O5 | 129.0186, 103.0376 | ＋ | ＋ | - | Fr1 |
| C17 | Galloylglucose | 5.39 | 331.0655 | C13H16O10 | 211.0232, 169.0139, 151.0033, 125.0245 | ＋ | ＋ | ＋ | Zong |
| C18 | (Epi)Catechin trimers | 5.64 | 865.1871 | C45H38O18 | 739.1553, 713.1357, 695.1475, 577.1318, 451.0959, 407.0704, 287.0516 | ＋ | - | - | Zong |
| C19 | Hydroxyhydroquinone or Phloroglucinol or 1,2,3-Trihydroxybenzene | 6.42 | 125.0247 | C6H6O3 | 107.0133 | ＋ | ＋ | ＋ | Zong |
| C20 | Gallic acid | 7.02 | 169.0166 | C7H6O5 | 125.0247 | ＋ | ＋ | ＋ | Zong |
| C21 | Hydroxyhydroquinone or Phloroglucinol or 1,2,3-Trihydroxybenzene | 7.02 | 125.0283 | C6H6O3 | 107.0150 | ＋ | ＋ | ＋ | Zong |
| C22 | 2/6/1'/4'/6'-*O*-Galloylsucrose | 7.39 | 493.1161 | C19H26O15 | 331.0673, 169.0135, 125.0233 | ＋ | ＋ | ＋ | Zong |
| C23 | Phenylalanine | 7.78 | 164.0717 | C9H11NO2 | 147.0451, 103.0558 | ＋ | ＋ | ＋ | Zong |
| C24 | 2/6/1'/4'/6'-*O*-Galloylsucrose | 7.81 | 493.1173 | C19H26O15 | 331.0676, 169.0134, 125.0236 | ＋ | ＋ | ＋ | Zong |
| C25 | Methoxy-galloylglucose | 8.38 | 345.0797 | C14H18O10 | 183.0286, 168.0067 | ＋ | - | ＋ | Fr1 |
| C26 | Gallocatechin or its isomer | 8.63 | 305.0645 | C15H14O7 | 179.0337, 137.0261, 125.0235 | ＋ | - | - | Zong |
| C27 | 1,2-di-*O*-galloyl-*β*-D-glucose or 1,6-di-*O*-galloyl-*β*-D-glucose or its isomer | 8.96 | 483.0735 | C20H20O14 | 331.0626, 313.0546, 169.0137, 125.0248 | ＋ | - | - | Zong |
| C28 | Hydroxyhydroquinone or Phloroglucinol or 1,2,3-Trihydroxybenzene | 9.19 | 125.0247 | C6H6O3 | 107.0144 | ＋ | ＋ | ＋ | Zong |
| C29 | (+)-Catechin or Epicatechin or its isomer | 9.21 | 289.0708 | C15H14O6 | 271.0577, 245.0807, 205.0485, 179.0335, 125.0243 | ＋ | ＋ | ＋ | Zong |
| C30 | (Epi)Catechin glucoside | 9.21 | 451.1242 | C21H24O11 | 313.0691, 289.0707, 271.0629, 245.0780, 137.0246 | ＋ | ＋ | ＋ | Zong |
| C31 | Epicatechin-(4beta->8)-epicatechin-(4beta->8)-catechin 3/3'/3''-gallate | 9.39 | 1017.2032 | C52H42O22 | 577.1347, 407.0819, 289.0672, 125.0241 | ＋ | - | - | Zong |
| C32 | (Epi)Catechin dimers | 10.15 | 577.1374 | C30H26O12 | 451.1034, 425.0814, 289.0709, 245.0812, 125.0243 | ＋ | - | - | Zong |
| C33 | (Epi)Catechin trimers | 10.45 | 865.1879 | C45H38O18 | 739.1594, 713.1444, 695.1390, 577.1372, 451.0921, 407.0825, 287.0599 | ＋ | - | - | Zong |
| C34 | Methoxy-galloylglucose | 10.46 | 345.0804 | C14H18O10 | 183.0280, 168.0090 | ＋ | ＋ | ＋ | Fr1 |
| C35 | (Epi)Catechin dimers | 10.53 | 577.1379 | C30H26O12 | 451.0986, 425.0849, 289.0713, 245.0792, 125.0243 | ＋ | - | - | Zong |
| C36 | Coumaric acid glucoside | 10.62 | 325.0908 | C15H18O8 | 265.0657, 145.0296, 119.0495, 117.0339 | ＋ | ＋ | ＋ | Zong |
| C37 | Benzenedicarboxylic acid | 10.73 | 165.0187 | C8H6O4 | 121.0300 | ＋ | ＋ | ＋ | Fr2 |
| C38 | (+)-Catechin or Epicatechin or its isomer | 10.73 | 289.0717 | C15H14O6 | 271.0577, 245.0830, 205.0502, 179.0322, 125.0249 | ＋ | ＋ | ＋ | Zong |
| C39 | (Epi)Catechin glucoside | 10.77 | 451.1264 | C21H24O11 | 313.0694, 289.0702, 271.0649, 245.0811, 137.0244 | ＋ | ＋ | ＋ | Zong |
| C40 | 1,2-di-*O*-galloyl-*β*-D-glucose or 1,6-di-*O*-galloyl-*β*-D-glucose or its isomer | 10.78 | 483.0734 | C20H20O14 | 331.0689, 313.0556, 169.0163, 125.0230 | ＋ | - | - | Fr2 |
| C41 | Tryptophan | 11.17 | 203.0824 | C11H12N2O2 | 159.0939, 116.0512 | ＋ | ＋ | - | Zong |
| C42 | (Epi)Catechin trimers | 11.35 | 865.1872 | C45H38O18 | 739.1445, 713.1368, 695.1337, 577.1420, 451.0951, 407.0750, 287.0514 | ＋ | - | - | Zong |
| C43 | Epicatechin-(4beta->8)-epicatechin-(4beta->8)-catechin 3/3'/3''-gallate | 11.35 | 1017.1922 | C52H42O22 | 577.1265, 407.0762, 289.0731, 125.0259 | ＋ | - | - | Zong |
| C44 | Coumaric acid glucoside | 11.35 | 325.0914 | C15H18O8 | 265.0705, 145.0287, 119.0506, 117.0346 | ＋ | ＋ | ＋ | Zong |
| C45 | Methoxy-galloylglucose | 11.53 | 345.0804 | C14H18O10 | 183.0279, 168.0067 | ＋ | ＋ | ＋ | Fr1 |
| C46 | 1,2-di-*O*-galloyl-*β*-D-glucose or 1,6-di-*O*-galloyl-*β*-D-glucose or its isomer | 11.53 | 483.0728 | C20H20O14 | 331.0667, 313.0569, 169.0146, 125.0237 | ＋ | ＋ | - | Zong |
| C47 | Benzenedicarboxylic acid | 11.67 | 165.0185 | C8H6O4 | 121.0306 | ＋ | ＋ | ＋ | Fr2 |
| C48 | *O*-Methylgallic acid | 11.98 | 183.0297 | C8H8O5 | 168.0061, 139.0415, 124.0152 | ＋ | ＋ | ＋ | Zong |
| C49 | Epicatechin-(4beta->8)-epicatechin-(4beta->8)-catechin 3/3'/3''-gallate | 11.98 | 1017.2002 | C52H42O22 | 577.1299, 407.0715, 289.0677, 125.0257 | ＋ | - | - | Zong |
| C50 | (Epi)Catechin glucoside | 12.08 | 451.1264 | C21H24O11 | 313.0522, 289.0694, 271.0640, 245.1000, 137.0239 | ＋ | ＋ | ＋ | Zong |
| C51 | (Epi)Catechin dimers | 12.17 | 577.1318 | C30H26O12 | 451.0935, 425.0828, 289.0692, 245.0812, 125.0248 | ＋ | - | - | Zong |
| C52 | Benzenedicarboxylic acid | 12.32 | 165.0188 | C8H6O4 | 121.0303 | ＋ | ＋ | ＋ | Zong |
| C53 | (+)-Catechin or Epicatechin or its isomer | 12.32 | 289.0720 | C15H14O6 | 245.0810, 205.0508, 179.0349, 125.0236 | ＋ | ＋ | ＋ | Zong |
| C54 | Coumaric acid glucoside | 12.48 | 325.0912 | C15H18O8 | 265.0700, 145.0293, 119.0501, 117.0343 | ＋ | ＋ | ＋ | Zong |
| C55 | 6-hydroxymusizin-8-*O*-*β*-D-glucopyranoside or its isomer | 12.48 | 393.1155 | C19H22O9 | 231.0641, 189.0575 | ＋ | ＋ | - | Zong |
| C56 | 1,2-di-*O*-galloyl-*β*-D-glucose or 1,6-di-*O*-galloyl-*β*-D-glucose or its isomer | 12.53 | 483.0733 | C20H20O14 | 331.0772, 313.0599, 169.0139, 125.0240 | ＋ | - | ＋ | Zong |
| C57 | (Epi)Catechin trimers | 12.64 | 865.1877 | C45H38O18 | 739.1485, 713.1447, 695.1304, 577.1265, 451.1004, 407.0735, 287.0536 | ＋ | - | - | Zong |
| C58 | Methyl gallate | 12.82 | 183.0292 | C8H8O5 | 168.0093, 124.0152 | ＋ | ＋ | ＋ | Zong |
| C59 | Epicatechin-(4beta->8)-epicatechin-(4beta->8)-catechin 3/3'/3''-gallate | 12.89 | 1017.1964 | C52H42O22 | 577.1325, 407.0825, 289.0702, 125.0257 | ＋ | - | - | Zong |
| C60 | (Epi)Catechin dimers gallate | 12.89 | 729.1441 | C37H30O16 | 577.1292, 407.0729, 289.0699, 169.0133, 125.0248 | ＋ | - | - | Zong |
| C61 | Homogentisic acid | 13.02 | 167.0341 | C8H8O4 | 123.0447, 108.0239 | ＋ | ＋ | ＋ | Zong |
| C62 | Gallocatechin or its isomer | 13.12 | 305.0648 | C15H14O7 | 179.0323, 137.0246, 125.0249 | ＋ | - | - | Zong |
| C63 | Epicatechin-(4beta->8)-epicatechin-(4beta->8)-catechin 3/3'/3''-gallate | 13.25 | 1017.1967 | C52H42O22 | 577.1340, 407.0792, 289.0681, 125.0239 | ＋ | - | - | Zong |
| C64 | (Epi)Catechin dimers gallate | 13.25 | 729.1438 | C37H30O16 | 577.1340, 407.0729, 289.0699, 169.0133, 125.0248 | ＋ | - | - | Zong |
| C65 | Coumaric acid glucoside | 13.25 | 325.0920 | C15H18O8 | 265.0684, 145.0296, 119.0508, 117.0349 | ＋ | ＋ | ＋ | Zong |
| C66 | (+)-Catechin or Epicatechin or its isomer | 13.46 | 289.0712 | C15H14O6 | 245.0800, 205.0503, 179.0340, 125.0233 | ＋ | - | - | Zong |
| C67 | (Epi)Catechin dimers | 13.76 | 577.1325 | C30H26O12 | 451.1089, 425.0858, 289.0723, 245.0806, 125.0237 | ＋ | - | - | Zong |
| C68 | 6-hydroxymusizin-8-*O*-*β*-D-glucopyranoside or its isomer | 13.76 | 393.1169 | C19H22O9 | 231.0644, 189.0537 | ＋ | ＋ | ＋ | Zong |
| C69 | 1,2-di-*O*-galloyl-*β*-D-glucose or 1,6-di-*O*-galloyl-*β*-D-glucose or its isomer | 13.97 | 483.0736 | C20H20O14 | 331.0650, 313.0537, 169.0129, 125.0224 | ＋ | ＋ | ＋ | Zong |
| C70 | Tri-*O*-galloyl-glucose | 13.97 | 635.0874 | C27H24O18 | 465.0617, 313.0573, 169.0129 | ＋ | - | - | Zong |
| C71 | (Epi)Catechin dimers gallate | 14.12 | 729.1423 | C37H30O16 | 577.1300, 407.0776, 289.0687, 169.0127, 125.0228 | ＋ | - | - | Zong |
| C72 | Epicatechin-(4beta->8)-epicatechin-(4beta->8)-catechin 3/3'/3''-gallate | 14.21 | 1017.1964 | C52H42O22 | 577.1325, 407.0692, 289.0680, 125.0248 | ＋ | - | - | Zong |
| C73 | Procyanidin B2 3,3'-di-*O*-gallate | 14.21 | 881.1517 | C44H34O20 | 729.1448, 559.1256, 541.1026, 407.0750, 289.0695, 169.0145, 125.0245 | ＋ | - | - | Zong |
| C74 | Coumaric acid glucoside | 14.29 | 325.0920 | C15H18O8 | 265.0704, 145.0295, 119.0495, 117.0348 | ＋ | ＋ | ＋ | Zong |
| C75 | (Epi)Catechin trimers | 14.45 | 865.1883 | C45H38O18 | 739.1574, 713.1353, 695.1352, 577.1237, 451.1009, 407.0740, 287.0525 | ＋ | ＋ | - | Fr2 |
| C76 | Methyl gallate | 14.50 | 183.0300 | C8H8O5 | 168.0066, 124.0158 | ＋ | ＋ | ＋ | Fr2 |
| C77 | (+)-Catechin or Epicatechin or its isomer | 14.68 | 289.0729 | C15H14O6 | 245.0803, 205.0483, 179.0329, 125.0238 | ＋ | ＋ | ＋ | Zong |
| C78 | Epicatechin-(4beta->8)-epicatechin-(4beta->8)-catechin 3/3'/3''-gallate | 14.90 | 1017.1967 | C52H42O22 | 577.1382, 407.0738, 289.0699, 125.0235 | ＋ | - | - | Zong |
| C79 | Caffeic acid | 14.95 | 179.0345 | C9H8O4 | 135.0454, 107.0505 | ＋ | ＋ | ＋ | Zong |
| C80 | Phlorizin | 13.90 | 435.1217 | C21H24O10 | 273.0754, 167.0322 | ＋ | ＋ | - | Zong |
| C81 | Phlorizin isomer | 14.50 | 435.1258 | C21H24O10 | 273.0749, 167.0325 | ＋ | ＋ | ＋ | Fr1 |
| C82 | 2-(2'-hydroxypropyl)-5-methyl-7-hydroxychromone or its isomer | 15.15 | 233.0805 | C13H14O4 | 189.0542, 149.0228, 105.0348 | ＋ | ＋ | ＋ | Zong |
| C83 | (Epi)Catechin dimers gallate | 15.32 | 729.1385 | C37H30O16 | 577.1268, 407.0727, 289.0660, 169.0137, 125.0249 | ＋ | - | - | Zong |
| C84 | 6-*O*-galloyl-1-*O*-*p*-coumaroyl-*β*-D-glucose or 1-*O*-galloyl-6-*O*-*p*-coumaroyl-*β*-D-glucose or its isomer | 15.32 | 477.1033 | C22H22O12 | 313.0543, 169.0137, 125.0236 | ＋ | ＋ | ＋ | Zong |
| C85 | Coumaric acid glucoside | 15.32 | 325.0906 | C15H18O8 | 265.0708, 145.0281, 119.0516, 117.0347 | ＋ | ＋ | ＋ | Zong |
| C86 | Epicatechin-3-*O*-gallate or 7-Galloylcatechin or their isomer | 15.51 | 441.0839 | C22H18O10 | 289.0702, 271.0599, 169.0139, 125.0240 | ＋ | - | - | Fr2 |
| C87 | 6-*O*-galloyl-1-*O*-*p*-coumaroyl-*β*-D-glucose or 1-*O*-galloyl-6-*O*-*p*-coumaroyl-*β*-D-glucose or its isomer | 15.73 | 477.1020 | C22H22O12 | 313.0664, 169.0138, 125.0241 | ＋ | ＋ | ＋ | Zong |
| C88 | (Epi)Catechin glucoside | 15.92 | 451.1194 | C21H24O11 | 313.0543, 289.0784, 271.0459, 245.0806, 137.0244 | ＋ | ＋ | ＋ | Fr2 |
| C89 | Tri-*O*-galloyl-glucose | 16.16 | 635.0830 | C27H24O18 | 465.0613, 313.0620, 169.0152 | ＋ | - | - | Fr2 |
| C90 | (+)-Catechin or Epicatechin or its isomer | 16.34 | 289.0703 | C15H14O6 | 271.0571, 245.0795, 205.0505, 179.0340, 125.0246 | ＋ | - | - | Zong |
| C91 | Epicatechin-3-*O*-gallate or 7-Galloylcatechin or their isomer | 16.34 | 441.0814 | C22H18O10 | 289.0711, 271.0599, 169.0106, 125.0274 | ＋ | ＋ | ＋ | Zong |
| C92 | 6-hydroxymusizin-8-*O*-*β*-D-glucopyranoside or its isomer | 16.42 | 393.1148 | C19H22O9 | 231.0656, 189.0536 | ＋ | - | - | Zong |
| C93 | Emodin 1-*O*-*β*-D-glucopyranoside isomer or Emodin 8-*O*-*β*-D-glucopyranoside isomer | 16.85 | 431.0960 | C21H20O10 | 269.0436, 225.0527 | ＋ | ＋ | ＋ | Fr2 |
| C94 | Quercetin or its isomer | 16.95 | 301.0339 | C15H10O7 | 151.004, 121.0309 | ＋ | ＋ | ＋ | Fr3 |
| C95 | Lindleyin | 17.22 | 477.1383 | C23H26O11 | 313.0540, 169.0141, 125.0242 | ＋ | ＋ | ＋ | Zong |
| C96 | 6-*O*-galloyl-1-*O*-*p*-coumaroyl-*β*-D-glucose or 1-*O*-galloyl-6-*O*-*p*-coumaroyl-*β*-D-glucose or its isomer | 17.22 | 477.1020 | C22H22O12 | 313.0530, 169.0132, 125.0229 | ＋ | ＋ | ＋ | Zong |
| C97 | Epicatechin-3-O-gallate or 7-Galloylcatechin or their isomer | 17.33 | 441.0790 | C22H18O10 | 289.0698, 271.0589, 169.0133, 125.0249 | ＋ | ＋ | ＋ | Zong |
| C98 | Cinnamic acid | 17.33 | 147.0451 | C9H8O2 | 103.0556 | ＋ | ＋ | ＋ | Zong |
| C99 | Coumalic acid | 17.87 | 163.0398 | C9H8O3 | 119.0503 | ＋ | ＋ | ＋ | Zong |
| C100 | Chrysophanol-*O*-glucopyranoside | 17.87 | 415.1016 | C21H20O9 | 253.0495, 225.0529 | ＋ | ＋ | - | Zong |
| C101 | 2-(2'-hydroxypropyl)-5-methyl-7-hydroxychromone or its isomer | 18.01 | 233.0808 | C13H14O4 | 189.0562, 149.0241, 105.0334 | ＋ | ＋ | ＋ | Fr2 |
| C102 | 6-*O*-galloyl-1-*O*-*p*-coumaroyl-*β*-D-glucose or 1-*O*-galloyl-6-*O*-*p*-coumaroyl-*β*-D-glucose or its isomer | 18.01 | 477.1017 | C22H22O12 | 313.0574, 169.0132, 125.0246 | ＋ | ＋ | ＋ | Fr2 |
| C103 | 1,2-di-*O*-galloyl-6-*O*-*p*-coumaroyl-*β*-D-glucose or 1,6-di-*O*-galloyl-2-*O*-*p*-coumaroyl-*β*-D-glucose or 2,6-di-*O*-galloyl-1-*O*-*p*-coumaroyl-*β*-D-glucose or its isomer | 18.04 | 629.1118 | C29H26O16 | 313.0548, 169.0145, 125.0254 | ＋ | - | - | Zong |
| C104 | 1,2-di-*O*-galloyl-6-*O*-*p*-coumaroyl-*β*-D-glucose or 1,6-di-*O*-galloyl-2-*O*-*p*-coumaroyl-*β*-D-glucose or 2,6-di-*O*-galloyl-1-*O*-*p*-coumaroyl-*β*-D-glucose or its isomer | 18.44 | 629.1071 | C29H26O16 | 313.0573, 169.0126, 125.0247 | ＋ | - | - | Zong |
| C105 | Epicatechin-3-*O*-gallate or 7-Galloylcatechin or their isomer | 18.64 | 441.0791 | C22H18O10 | 289.0688, 271.0584, 169.0188, 125.0251 | ＋ | - | - | Fr2 |
| C106 | 6-*O*-galloyl-1-*O*-*p*-coumaroyl-*β*-D-glucose or 1-*O*-galloyl-6-*O*-*p*-coumaroyl-*β*-D-glucose or its isomer | 18.73 | 477.0992 | C22H22O12 | 313.0520, 169.0137, 125.0239 | ＋ | ＋ | ＋ | Zong |
| C107 | Aloe-emodin 8-*O*-*β*-D-glucopyranoside | 19.23 | 431.0971 | C21H20O10 | 269.0417, 240.0410 | ＋ | ＋ | ＋ | Zong |
| C108 | Aloe-emodin isomer | 19.23 | 269.0442 | C15H10O5 | 239.0337 | ＋ | ＋ | ＋ | Zong |
| C109 | 1-*O*-galloyl-6-*O*-cinnamoyl-*β*-D-glucose or 2-*O*-galloyl-1-*O*-cinnamoyl-*β*-D-glucose or 1-*O*-galloyl-2-*O*-cinnamoyl-*β*-D-glucose | 19.39 | 461.1094 | C22H22O11 | 313.0538, 271.0453, 211.0230, 169.0134, 147.0444 | ＋ | ＋ | ＋ | Zong |
| C110 | Sennoside C or D or their isomer | 19.50 | 847.2058 | C42H40O19 | 685.1526, 431.0979, 386.0999, 269.0482, 224.0453 | ＋ | - | - | Fr2 |
| C111 | Stilbene | 19.65 | 417.1154 | C21H22O9 | 255.0651, 227.0676 | ＋ | - | - | Zong |
| C112 | Emodin Anthrone or its isomer | 19.71 | 255.0655 | C15H12O4 | 213.0556, 171.0423, 145.0660 | ＋ | - | - | Zong |
| C113 | 1,2-di-*O*-galloyl-6-*O*-*p*-coumaroyl-*β*-D-glucose or 1,6-di-*O*-galloyl-2-*O*-*p*-coumaroyl-*β*-D-glucose or 2,6-di-*O*-galloyl-1-*O*-*p*-coumaroyl-*β*-D-glucose or its isomer | 19.74 | 629.1113 | C29H26O16 | 313.0520, 169.0135, 125.0243 | ＋ | ＋ | - | Zong |
| C114 | Sennoside C or D or their isomer | 19.86 | 847.2061 | C42H40O19 | 685.1517, 431.0882, 386.1006, 269.0404, 224.0417 | ＋ | - | - | Zong |
| C115 | Sennoside C or D or their isomer | 20.37 | 847.2040 | C42H40O19 | 685.1512, 431.0898, 386.0988, 269.0426, 224.0462 | ＋ | - | - | Zong |
| C116 | 1,2-di-*O*-galloyl-6-*O*-*p*-coumaroyl-*β*-D-glucose or 1,6-di-*O*-galloyl-2-*O*-*p*-coumaroyl-*β*-D-glucose or 2,6-di-*O*-galloyl-1-*O*-*p*-coumaroyl-*β*-D-glucose or its isomer | 20.46 | 629.1070 | C29H26O16 | 313.0594, 169.0144, 125.0240 | ＋ | - | - | Fr2 |
| C117 | Chrysophanol-*O*-glucopyranoside | 20.59 | 415.1015 | C21H20O9 | 253.0494, 225.0561 | ＋ | ＋ | - | Zong |
| C118 | Quercetin or its isomer | 20.75 | 301.0344 | C15H10O7 | 151.0057, 121.0284 | ＋ | - | - | Fr3 |
| C119 | Aloe-emodin 1-*O*-*β*-D-glucopyranoside | 20.83 | 431.0988 | C21H20O10 | 269.0442, 240.0407 | ＋ | ＋ | ＋ | Fr2 |
| C120 | Sennoside B | 20.83 | 861.1853 | C42H38O20 | 699.1248, 386.0975, 224.0459 | ＋ | - | - | Zong |
| C121 | Stilbene | 20.83 | 417.1154 | C21H22O9 | 255.0656, 227.0684 | ＋ | ＋ | ＋ | Zong |
| C122 | Emodin Anthrone or its isomer | 20.94 | 255.0658 | C15H12O4 | 213.0554, 171.0463, 145.0657 | ＋ | ＋ | ＋ | Zong |
| C123 | 1-*O*-galloyl-6-*O*-cinnamoyl-*β*-D-glucose or 2-*O*-galloyl-1-*O*-cinnamoyl-*β*-D-glucose or 1-*O*-galloyl-2-*O*-cinnamoyl-*β*-D-glucose | 21.06 | 461.1098 | C22H22O11 | 313.0567, 271.0424, 211.0266, 169.0142, 147.0448 | ＋ | - | ＋ | Zong |
| C124 | 6-hydroxymusizin-8-*O*-*β*-D-glucopyranoside or its isomer | 21.18 | 393.1156 | C19H22O9 | 231.0651, 189.0517 | ＋ | ＋ | ＋ | Zong |
| C125 | Sennoside C or D or their isomer | 21.29 | 847.2040 | C42H40O19 | 685.1512, 431.0851, 386.0985, 269.0406, 224.0465 | ＋ | - | - | Zong |
| C126 | Chrysazin | 21.40 | 239.0343 | C14H8O4 | 211.0383, 183.0449 | ＋ | ＋ | ＋ | Zong |
| C127 | Rhein isomer | 21.47 | 283.0234 | C15H8O6 | 239.0310, 211.0377, 183.0436 | ＋ | ＋ | ＋ | Zong |
| C128 | Rhein 8-*O*-*β*-D-glucopyranoside | 21.47 | 445.0767 | C21H18O11 | 283.0247, 239.0338, 211.0373, 183.0461 | ＋ | ＋ | ＋ | Zong |
| C129 | 1,6-di-*O*-galloyl-2-*O*-cinnamoyl-*β*-D-glucose or 1,2-di-*O*-galloyl-6-*O*-cinnamoyl-*β*-D-glucose or 2,6-di-*O*-galloyl-1-*O*-cinnamoyl-*β*-D-glucose | 21.67 | 613.1170 | C29H26O15 | 465.0695, 313.0634, 211.0245, 169.0148 | ＋ | ＋ | ＋ | Zong |
| C130 | 2-(2'-hydroxypropyl)-5-methyl-7-hydroxychromone or its isomer | 21.82 | 233.0808 | C13H14O4 | 215.0676, 189.0568, 149.0238, 105.0332 | ＋ | ＋ | ＋ | Zong |
| C131 | Aloe-emodin 1-*O*-*β*-D-glucopyranoside isomer or Aloe-emodin 8-*O*-*β*-D-glucopyranoside isomer | 21.86 | 431.0939 | C21H20O10 | 269.0450, 240.0411 | ＋ | ＋ | ＋ | Fr2 |
| C132 | 1,2-di-*O*-galloyl-6-*O*-*p*-coumaroyl-*β*-D-glucose or 1,6-di-*O*-galloyl-2-*O*-*p*-coumaroyl-*β*-D-glucose or 2,6-di-*O*-galloyl-1-*O*-*p*-coumaroyl-*β*-D-glucose or its isomer | 22.10 | 629.1074 | C29H26O16 | 313.0552, 169.0140, 125.0245 | ＋ | ＋ | ＋ | Zong |
| C133 | 1,6-di-*O*-galloyl-2-*O*-cinnamoyl-*β*-D-glucose or 1,2-di-*O*-galloyl-6-*O*-cinnamoyl-*β*-D-glucose or 2,6-di-*O*-galloyl-1-*O*-cinnamoyl-β-D-glucose | 22.10 | 613.1167 | C29H26O15 | 465.0652, 313.0578, 211.0222, 169.0123 | ＋ | ＋ | ＋ | Zong |
| C134 | Emodin 8-*O*-*β*-D-(6’-*O*-Malonylglucoside) or Emodin 1-*O*-*β*-D-(6’-*O*-Malonylglucoside) | 22.20 | 517.0933 | C24H22O13 | 473.1058, 311.0549, 269.0406, 225.0553 | ＋ | ＋ | - | Zong |
| C135 | 1-*O*-galloyl-6-*O*-cinnamoyl-*β*-D-glucose or 2-*O*-galloyl-1-*O*-cinnamoyl-*β*-D-glucose or 1-*O*-galloyl-2-O-cinnamoyl-*β*-D-glucose | 22.54 | 461.1144 | C22H22O11 | 313.0550, 271.0447, 211.0243, 169.0136, 147.0448 | ＋ | ＋ | ＋ | Zong |
| C136 | Sennoside A | 22.83 | 861.1850 | C42H38O20 | 699.1333, 386.0977, 224.0463 | ＋ | - | - | Zong |
| C137 | 1,6-di-*O*-galloyl-2-*O*-cinnamoyl-*β*-D-glucose or 1,2-di-*O*-galloyl-6-*O*-cinnamoyl-*β*-D-glucose or 2,6-di-*O*-galloyl-1-*O*-cinnamoyl-*β*-D-glucose | 23.31 | 613.1131 | C29H26O15 | 313.0623, 211.0240, 169.0130 | ＋ | - | ＋ | Zong |
| C138 | 5, 5'-bis(*β*-D-glucopyranosyloxy) rheidin B or its isomer | 23.41 | 831.2031 | C42H40O18 | 669.1582, 386.0952, 269.0454, 224.0500 | ＋ | - | - | Zong |
| C139 | Stilbene | 23.61 | 417.1150 | C21H22O9 | 255.0643, 227.0727 | ＋ | - | - | Zong |
| C140 | Emodin 1-*O*-*β*-D-glucopyranoside | 24.22 | 431.1006 | C21H20O10 | 269.0446, 225.0560 | ＋ | ＋ | ＋ | Zong |
| C141 | 5, 5'-bis(*β*-D-glucopyranosyloxy) rheidin B or its isomer | 24.22 | 831.2097 | C42H40O18 | 669.1501, 386.1000, 269.0426, 224.0465 | ＋ | - | - | Zong |
| C142 | Rhein isomer | 24.35 | 283.0237 | C15H8O6 | 239.0351, 211.0389, 183.0440 | ＋ | - | - | Zong |
| C143 | Rhein derivative | 24.35 | 487.0827 | C23H20O12 | 283.0221, 239.0324 | ＋ | - | - | Fr2 |
| C144 | Torachrysone or its isomer | 24.49 | 245.0833 | C14H14O4 | 230.0572, 215.0331, 159.0433 | ＋ | ＋ | ＋ | Zong |
| C145 | Torachrysone 8-*O*-*β*-D-glucopyranoside | 24.49 | 407.1381 | C20H24O9 | 245.0794, 230.0575, 215.0394, 159.0450, 131.0499 | ＋ | ＋ | ＋ | Zong |
| C146 | Resveratrol 4'-*O*-*β*-D-glucopyranoside | 24.79 | 389.1216 | C20H22O8 | 227.0711, 185.0654 | ＋ | - | - | Zong |
| C147 | Quercetin or its isomer | 25.03 | 301.0355 | C15H10O7 | 178.9996, 151.0034, 121.0282 | ＋ | ＋ | ＋ | Zong |
| C148 | Stilbene | 25.41 | 449.1407 | C22H25O10 | 245.0794 | ＋ | ＋ | ＋ | Zong |
| C149 | Torachrysone or its isomer | 25.42 | 245.0800 | C14H14O4 | 230.0547, 215.0341, 159.0435 | ＋ | - | - | Zong |
| C150 | 5, 5'-bis(*β*-D-glucopyranosyloxy) rheidin B or its isomer | 25.42 | 831.2106 | C42H40O18 | 669.1493, 386.0922, 269.0427, 224.0466 | ＋ | - | - | Zong |
| C151 | Chrysophanol isomer | 25.59 | 253.0499 | C15H10O4 | 225.0567 | ＋ | - | - | Fr2 |
| C152 | 5, 5'-bis(*β*-D-glucopyranosyloxy) rheidin B or its isomer | 26.00 | 831.2014 | C42H40O18 | 669.1499, 386.0965, 269.0453, 224.0454 | ＋ | - | - | Zong |
| C153 | Rhein derivative | 26.08 | 487.0828 | C23H20O12 | 283.0229, 239.0337 | ＋ | ＋ | ＋ | Zong |
| C154 | Chrysophanol-*O*-glucopyranoside | 26.49 | 415.1028 | C21H20O9 | 253.0501, 225.0550 | ＋ | ＋ | ＋ | Zong |
| C155 | Chrysophanol isomer | 26.53 | 253.0500 | C15H10O4 | 225.0556 | ＋ | ＋ | ＋ | Zong |
| C156 | Stilbene | 26.93 | 449.1420 | C22H25O10 | 245.0806 | ＋ | ＋ | ＋ | Fr3 |
| C157 | Torachrysone or its isomer | 26.99 | 245.0810 | C14H14O4 | 230.0576, 215.0339, 159.0452 | ＋ | ＋ | ＋ | Zong |
| C158 | Chrysophanol-*O*-glucopyranoside | 27.04 | 415.1015 | C21H20O9 | 253.0500, 225.0561 | ＋ | ＋ | ＋ | Zong |
| C159 | Chrysophanol isomer | 27.05 | 253.0502 | C15H10O4 | 225.0553 | ＋ | ＋ | ＋ | Zong |
| C160 | Torachrysone or its isomer | 27.50 | 245.0810 | C14H14O4 | 230.0582, 215.0352, 159.0451 | ＋ | - | - | Fr2 |
| C161 | Emodin 8-*O*-*β*-D-glucopyranoside | 27.71 | 431.1004 | C21H20O10 | 269.0432, 225.0553 | ＋ | ＋ | ＋ | Zong |
| C162 | Emodin isomer | 27.71 | 269.0448 | C15H10O5 | 225.0550 | ＋ | ＋ | ＋ | Fr3 |
| C163 | Chrysophanol isomer | 28.33 | 253.0497 | C15H10O4 | 225.0531 | ＋ | ＋ | ＋ | Fr3 |
| C164 | Chrysophanol isomer | 29.14 | 253.0513 | C15H10O4 | 225.0551 | ＋ | ＋ | ＋ | Fr3 |
| C165 | Chrysophanol | 29.59 | 253.0502 | C15H10O4 | 225.054 | ＋ | ＋ | ＋ | Fr3 |
| C166 | Emodin 8-*O*-*β*-D-(6’-O-Malonylglucoside) or Emodin 1-*O*-*β*-D-(6’-O-Malonylglucoside) | 29.66 | 517.0912 | C24H22O13 | 473.1048, 311.0545, 269.0436, 225.0540 | ＋ | - | - | Zong |
| C167 | Stilbene | 29.69 | 449.1407 | C22H25O10 | 245.0804 | ＋ | ＋ | ＋ | Zong |
| C168 | Physcion isomer | 29.81 | 283.0610 | C16H12O5 | 240.0416 | ＋ | ＋ | ＋ | Zong |
| C169 | Physcion 8-*O*-*β*-D-glucopyranoside or its isomer | 29.84 | 445.1119 | C22H22O10 | 283.0591, 240.0409 | ＋ | ＋ | ＋ | Zong |
| C170 | Physcion | 30.79 | 283.0605 | C16H12O5 | 240.0428 | ＋ | ＋ | ＋ | Zong |
| C171 | Physcion 8-*O*-*β*-D-glucopyranoside or its isomer | 30.85 | 445.1121 | C22H22O10 | 283.0596, 240.0401 | ＋ | ＋ | ＋ | Zong |
| C172 | Emodin 8-*O*-*β*-D-glucopyranoside | 31.06 | 431.0941 | C21H20O10 | 269.0424, 225.0543 | ＋ | ＋ | ＋ | Fr3 |
| C173 | Emodin isomer | 31.06 | 269.0468 | C15H10O5 | 225.0533 | ＋ | ＋ | ＋ | Fr3 |
| C174 | Citreorosein | 31.66 | 285.0400 | C15H10O6 | 241.0445, 211.0353 | ＋ | ＋ | ＋ | Fr3 |
| C175 | Physcion isomer | 32.39 | 283.0595 | C16H12O5 | 240.0414 | ＋ | - | - | Fr3 |
| C176 | Aloe-emodin | 32.76 | 269.0438 | C15H10O5 | 239.032 | ＋ | ＋ | ＋ | Zong |
| C177 | Chrysophanol isomer | 32.87 | 253.0508 | C15H10O4 | 225.0577 | ＋ | ＋ | ＋ | Fr3 |
| C178 | 6-Methylrhein | 32.98 | 297.0399 | C16H10O6 | 253.0493, 225.0516 | ＋ | ＋ | ＋ | Zong |
| C179 | Physcion isomer | 33.29 | 283.0592 | C16H12O5 | 240.0405 | ＋ | - | - | Zong |
| C180 | Physcion isomer | 35.76 | 283.0584 | C16H12O5 | 240.0405 | ＋ | ＋ | ＋ | Fr3 |
| C181 | Alizarin | 35.97 | 239.0341 | C14H8O4 | 211.0382, 183.0453 | ＋ | ＋ | ＋ | Zong |
| C182 | Rhein | 36.14 | 283.0234 | C15H8O6 | 239.0333, 211.0378, 183.0444 | ＋ | ＋ | ＋ | Zong |
| C183 | Emodin | 37.25 | 269.0456 | C15H10O5 | 225.0547 | ＋ | ＋ | ＋ | Zong |

Note: the red text represented the compounds that can only be identified by offline 2D LPLC/HPLC coupled with MS technology; Regardless of whether MS is combined with offline 2D LC separation, other compounds can be identified; Zong represented the rhubarb extracting solution without offline 2D LC separation.

**Supplementary Table 2** The identification results of the prototypes and metabolites in RR, SR and CR.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Num. | Name | RT (min) | [M-H]- | PPM | Formula | MS/MS | RR  -P | RR  -U | SR  -P | SR  -U | CR  -P | CR  -U |
| C1 | Gallic acid | 7.04 | 169.0138 | 3.85 | C7H6O5 | 125.0247 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C2 | Methylate-Gallic acid-*O*-GluA | 8.47 | 359.0577 | -8.04 | C14H16O11 | 183.0278, 124.0162 | ＋ | - | ＋ | + | ＋ | - |
| C3 | Methylate-Gallic acid | 9.01 | 183.0300 | 6.56 | C8H8O5 | 168.0066, 139.0390, 124.0145 | ＋ | - | - | - | - | - |
| C4 | Methylate-Gallic acid | 9.99 | 183.0295 | 3.83 | C8H8O5 | 168.0056, 139.0395, 124.0161 | ＋ | ＋ | ＋ | - | ＋ | - |
| C5 | Methylate-Gallic acid | 10.26 | 183.0294 | 3.28 | C8H8O5 | 168.0060, 139.0412, 124.0162 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C6 | Methylate-Gallic acid | 11.96 | 183.0295 | 3.83 | C8H8O5 | 168.0059, 139.0424, 124.0157 | ＋ | - | ＋ | - | ＋ | - |
| C7 | Methylate-Gallic acid | 12.23 | 183.0290 | 1.09 | C8H8O5 | 168.0060, 139.0415, 124.0163 | ＋ | - | ＋ | - | ＋ | - |
| C8 | Methylate-Gallic acid | 12.89 | 183.0299 | 6.01 | C8H8O5 | 168.0053, 124.0162 | - | - | - | ＋ | - | ＋ |
| C9 | Methylate-Gallic acid | 14.44 | 183.0300 | 6.56 | C8H8O5 | 168.0052, 124.0168 | - | + | ＋ | ＋ | ＋ | ＋ |
| C10 | Methylate-Gallic acid-*O*-SO3 | 10.33 | 262.9847 | -3.48 | C8H8SO8 | 183.0286, 168.0058, 124.0162 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C11 | Methylate-Gallic acid-*O*-SO3 | 14.41 | 262.9866 | 3.75 | C8H8SO8 | 183.0303, 168.0050, 124.0163 | - | ＋ | ＋ | ＋ | ＋ | ＋ |
| C12 | Dimethylate-Gallic acid-*O*-SO3 | 13.85 | 276.9997 | -5.65 | C9H10SO8 | 197.0440, 183.0261, 168.0012, 124.0122 | ＋ | ＋ | ＋ | ＋ | ＋ | - |
| C13 | Decarboxylate-Gallic acid | 7.04 | 125.0244 | 8.63 | C6H6O3 | - | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C14 | Decarboxylate-Gallic acid | 7.88 | 125.0243 | 7.83 | C6H6O3 | - | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C15 | Decarboxylate-Gallic acid | 8.83 | 125.0240 | 5.44 | C6H6O3 | - | - | ＋ | ＋ | ＋ | ＋ | ＋ |
| C16 | Decarboxylate-Gallic acid | 9.36 | 125.0243 | 7.83 | C6H6O3 | - | - | ＋ | - | ＋ | - | ＋ |
| C17 | Decarboxylate-Gallic acid | 11.27 | 125.0242 | 7.03 | C6H6O3 | - | - | - | - | ＋ | - | ＋ |
| C18 | Decarboxylate-Gallic acid-*O*-GluA | 6.83 | 301.0542 | -4.01 | C12H14O9 | 175.0244, 125.0248 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C19 | Gallic acid-*O*-GluA | 8.66 | 345.0427 | -7.35 | C13H14O11 | 169.0132, 125.0248 | ＋ | ＋ | ＋ | ＋ | ＋ | - |
| C20 | (Epi)catechin | 10.45 | 289.0694 | -4.38 | C15H14O6 | 271.0555, 245.0776 | ＋ | ＋ | ＋ | ＋ | ＋ | - |
| C21 | (Epi)catechin | 12.30 | 289.0722 | 5.31 | C15H14O6 | 271.0675, 245.0840 | ＋ | - | - | ＋ | - | + |
| C22 | Methylate-(Epi)catechin | 11.62 | 303.0871 | 2.59 | C16H16O6 | 285.0779, 259.0943 | ＋ | ＋ | - | - | - | - |
| C23 | Methylate-(Epi)catechin | 12.98 | 303.0844 | -6.32 | C16H16O6 | 285.0726, 259.0943 | ＋ | ＋ | ＋ | ＋ | ＋ | - |
| C24 | Methylate-(Epi)catechin | 14.29 | 303.0870 | 2.26 | C16H16O6 | 285.0708, 259.0948 | ＋ | ＋ | - | ＋ | - | - |
| C25 | Methylate-(Epi)catechin | 15.61 | 303.0875 | 3.91 | C16H16O6 | 285.0732, 259.0964 | - | ＋ | - | ＋ | - | ＋ |
| C26 | Methylate-(Epi)catechin-*O*-SO3 | 14.08 | 383.0393 | -10.00 | C16H16SO9 | 303.0837, 259.0929, 216.9814 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C27 | Methylate-(Epi)catechin-*O*-SO3 | 15.49 | 383.0388 | -11.30 | C16H16SO9 | 303.0820, 216.9839 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C28 | Methylate-(Epi)catechin-*O*-GluA | 11.63 | 479.1125 | -9.19 | C22H24O12 | 303.0847, 259.0936 | ＋ | ＋ | ＋ | ＋ | ＋ | - |
| C29 | Methylate-(Epi)catechin-*O*-GluA | 12.98 | 479.1146 | -7.94 | C22H24O12 | 303.0849, 259.0937 | ＋ | ＋ | ＋ | ＋ | ＋ | - |
| C30 | Methylate-(Epi)catechin-*O*-GluA | 14.32 | 479.1202 | 3.75 | C22H24O12 | 303.0878, 259.0981 | - | ＋ | - | ＋ | - | - |
| C31 | (Epi)catechin-*O*-GluA | 8.80 | 465.0984 | -9.36 | C21H22O12 | 289.0691, 245.0806 | ＋ | ＋ | ＋ | ＋ | ＋ | - |
| C32 | (Epi)catechin-*O*-GluA | 10.38 | 465.0999 | -6.13 | C21H22O12 | 289.0737, 245.0784 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C33 | (Epi)catechin-*O*-GluA | 12.49 | 465.0997 | -6.56 | C21H22O12 | 289.0686, 245.0779 | ＋ | ＋ | ＋ | ＋ | ＋ | - |
| C34 | (Epi)catechin-*O*-SO3 | 11.80 | 369.0255 | -5.36 | C15H14SO9 | 289.0678, 245.0872 | ＋ | ＋ | - | ＋ | - | ＋ |
| C35 | (Epi)catechin-*O*-SO3 | 22.56 | 369.0261 | -3.74 | C15H14SO9 | 289.0706, 245.0805 | - | - | ＋ | ＋ | - | - |
| C36 | Rhein | 36.00 | 283.0234 | -1.11 | C15H8O6 | 239.0307, 211.0374, 183.0438 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C37 | Rhein isomer | 21.61 | 283.0212 | -8.88 | C15H8O6 | 239.0309, 211.0368, 183.0452 | ＋ | ＋ | ＋ | - | ＋ | - |
| C38 | Rhein isomer | 23.63 | 283.0210 | -9.59 | C15H8O6 | 239.0324, 211.0376, 183.0449 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C39 | Hydroxyrhein | 25.49 | 299.0145 | -5.78 | C15H8O7 | 255.0260, 227.0310, 183.044 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C40 | Hydroxyrhein | 29.93 | 299.0191 | 1.58 | C15H8O7 | 255.0280, 227.0300, 211.0381 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C41 | Hydroxyrhein | 35.99 | 299.0194 | 2.58 | C15H8O7 | 255.0288, 227.0343, 211.0390 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C42 | Hydroxyrhein | 37.05 | 299.0180 | -2.10 | C15H8O7 | 255.0288, 227.0343, 211.0390 | - | ＋ | ＋ | ＋ | ＋ | ＋ |
| C43 | Rhein*-O*-SO3 | 23.50 | 362.9771 | -9.45 | C15H8SO9 | 283.0204, 239.0334, 211.0343, 183.0414 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C44 | Rhein*-O*-GluA | 21.56 | 459.0557 | -0.22 | C21H16O12 | 283.0199, 239.0293, 211.0442, 183.0435 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C45 | Hydroxyrhein-*O*-SO3 | 25.49 | 378.9759 | 1.21 | C15H8SO10 | 299.0140, 255.0261 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C46 | Hydroxyrhein-*O*-SO3 | 29.93 | 378.9748 | -1.70 | C15H8SO10 | 299.0153, 255.0271 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C47 | Methylate-Hydroxyrhein | 18.33 | 313.0345 | 0.71 | C16H10O7 | 233.0796, 189.0543 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C48 | Emodin | 37.25 | 269.0450 | 2.05 | C15H10O5 | 241.0466, 225.0526, 197.0591, 182.0368 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C49 | Emodin isomer | 18.34 | 269.0441 | -1.30 | C15H10O5 | 241.0489, 225.0533, 197.0559, 182.0387 | ＋ | - | ＋ | - | ＋ | - |
| C50 | Emodin isomer | 25.38 | 269.0431 | -5.02 | C15H10O5 | 241.0448, 225.0519, 197.0573, 182.0310 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C51 | Emodin isomer | 25.64 | 269.0462 | 6.51 | C15H10O5 | 241.0491, 225.0558, 197.0592, 182.0353 | - | ＋ | - | ＋ | + | ＋ |
| C52 | Emodin isomer | 26.31 | 269.0445 | 0.19 | C15H10O5 | 241.0475, 225.0525, 197.0622 | - | ＋ | - | ＋ | - | ＋ |
| C53 | Emodin isomer | 27.93 | 269.0443 | -0.56 | C15H10O5 | 241.0477, 225.0527, 197.0579, 182.0371 | ＋ | ＋ | ＋ | - | ＋ | - |
| C54 | Emodin isomer | 31.41 | 269.0452 | 2.79 | C15H10O5 | 241.0456, 225.0536, 197.0588, 182.0353 | ＋ | + | ＋ | - | ＋ | - |
| C55 | Carboxyemodin | 35.39 | 313.0348 | 1.66 | C16H10O7 | 269.0412, 225.0525 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C56 | Hydroxyemodin | 18.68 | 285.0399 | 1.88 | C15H10O6 | 241.0522, 211.0334 | ＋ | - | ＋ | - | ＋ | - |
| C57 | Hydroxyemodin | 22.54 | 285.0402 | 2.93 | C15H10O6 | 241.0413, 211.0375 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C58 | Hydroxyemodin | 25.73 | 285.0400 | 2.23 | C15H10O6 | 241.0463, 211.0369 | ＋ | - | ＋ | - | ＋ | + |
| C59 | Hydroxyemodin | 26.09 | 285.0397 | 1.18 | C15H10O6 | 241.0504, 211.0386 | - | ＋ | ＋ | ＋ | + | ＋ |
| C60 | Hydroxyemodin | 31.77 | 285.0406 | 4.34 | C15H10O6 | 241.0513, 211.0370 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C61 | Hydroxyemodin | 33.54 | 285.0401 | 2.58 | C15H10O6 | 241.0395, 211.0382 | ＋ | - | - | - | - | - |
| C62 | Hydroxyemodin | 35.29 | 285.0402 | 2.93 | C15H10O6 | 241.0414, 211.0373 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C63 | Hydroxyemodin*-O*-GluA | 22.60 | 461.0715 | 0.10 | C21H18O12 | 285.0351, 257.0409, 241.0453, 211.0353 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C64 | Hydroxyemodin*-O*-SO3 | 25.34 | 364.9969 | 1.98 | C15H10SO9 | 285.0360, 241.0469, 211.0371 | ＋ | - | ＋ | - | ＋ | - |
| C65 | Hydroxyemodin*-O*-SO3 | 26.02 | 364.9967 | 1.43 | C15H10SO9 | 285.0342, 241.0431, 211.0405 | ＋ | + | ＋ | + | ＋ | + |
| C66 | Emodin-*O*-GluA | 19.33 | 445.0744 | -4.80 | C21H18O11 | 269.0429, 241.0499 | ＋ | ＋ | ＋ | - | ＋ | - |
| C67 | Emodin-*O*-SO3 | 20.24 | 348.9989 | -6.78 | C21H18O11 | 269.0416, 241.0465, 225.0527 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C68 | Emodin-*O*-SO3 | 21.98 | 348.9979 | -9.64 | C15H10SO8 | 269.0416, 241.0465, 225.0498 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C69 | Emodin-*O*-SO3 | 30.06 | 348.9987 | -7.35 | C15H10SO8 | 269.0411, 241.0471, 225.0512 | ＋ | - | ＋ | + | ＋ | + |
| C70 | Emodin-*O*-SO3 | 32.05 | 348.9980 | -9.35 | C15H10SO8 | 269.0418, 241.0445, 225.0539 | ＋ | + | ＋ | + | ＋ | + |
| C71 | Emodin-*O*-SO3 | 36.08 | 348.9975 | -13.93 | C15H10SO8 | 269.0435, 241.0494, 225.0566 | + | - | - | - | - | - |
| C72 | Emodin-*O*-GluA-SO3 | 16.01 | 525.0341 | 1.42 | C21H18SO14 | 445.0796, 349.0013, 269.0406 | ＋ | ＋ | ＋ | - | ＋ | - |
| C73 | Emodin-*O*-GluA-SO3 | 18.33 | 525.0301 | -6.19 | C21H18SO14 | 445.0677, 348.9986, 269.0414, 225.0568 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C74 | Aloe-emodin | 31.96 | 269.0432 | -4.65 | C15H10O5 | 239.0321 | ＋ | - | ＋ | - | ＋ | - |
| C75 | Aloe-emodin isomer | 19.38 | 269.0424 | -7.62 | C15H10O5 | 239.0306 | ＋ | ＋ | ＋ | - | ＋ | - |
| C76 | Aloe-emodin isomer | 20.43 | 269.0431 | -5.02 | C15H10O5 | 239.0305 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C77 | Aloe-emodin isomer | 21.98 | 269.0429 | -5.76 | C15H10O5 | 239.0301 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C78 | Physcion | 30.52 | 283.0605 | 1.41 | C16H12O5 | 240.0455 | ＋ | ＋ | ＋ | - | ＋ | - |
| C79 | Physcion isomer | 31.59 | 283.0584 | -6.01 | C16H12O5 | 240.0375 | ＋ | ＋ | ＋ | - | ＋ | - |
| C80 | Physcion isomer | 32.86 | 283.0594 | -2.47 | C16H12O5 | 240.0416 | ＋ | ＋ | - | ＋ | - | ＋ |
| C81 | Physcion isomer | 36.42 | 283.0607 | 2.12 | C16H12O5 | 240.0400 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C82 | Hydroxyphyscion | 23.63 | 299.0546 | -1.39 | C16H12O6 | 256.0371 | ＋ | ＋ | ＋ | ＋ | - | ＋ |
| C83 | Hydroxyphyscion | 25.87 | 299.0539 | -3.73 | C16H12O6 | 256.0370 | - | ＋ | ＋ | ＋ | ＋ | ＋ |
| C84 | Hydroxyphyscion | 27.91 | 299.0547 | -1.05 | C16H12O6 | 256.0359 | - | ＋ | ＋ | ＋ | ＋ | - |
| C85 | Hydroxyphyscion | 31.50 | 299.0544 | -2.06 | C16H12O6 | 256.0370 | - | ＋ | - | - | - | - |
| C86 | Hydroxyphyscion | 34.37 | 299.0560 | 3.30 | C16H12O6 | 256.0357 | ＋ | - | ＋ | - | ＋ | - |
| C87 | Hydroxyphyscion | 34.98 | 299.0542 | -2.72 | C16H12O6 | 256.0355 | ＋ | ＋ | - | - | - | - |
| C88 | Hydroxyphyscion | 37.05 | 299.0554 | 1.29 | C16H12O6 | 256.0355 | - | ＋ | - | ＋ | - | ＋ |
| C89 | Hydroxyphyscion | 37.45 | 299.0533 | -5.73 | C16H12O6 | 256.0366 | - | ＋ | - | ＋ | - | ＋ |
| C90 | Physcion-*O*-GluA | 30.49 | 459.0901 | -4.55 | C22H20O11 | 283.0561, 240.0380 | ＋ | ＋ | ＋ | - | ＋ | - |
| C91 | Physcion-*O*-GluA | 31.63 | 459.0900 | -4.77 | C22H20O11 | 283.0552, 240.0364 | ＋ | ＋ | ＋ | - | ＋ | - |
| C92 | Physcion-*O*-SO3 | 33.77 | 363.0153 | -4.45 | C16H12SO8 | 283.0597, 240.0419 | - | ＋ | - | ＋ | - | ＋ |
| C93 | Physcion-*O*-SO3 | 21.67 | 363.0160 | -2.52 | C16H12SO8 | 283.0585, 240.0392 | - | ＋ | - | ＋ | - | ＋ |
| C94 | Physcion-*O*-SO3 | 20.88 | 363.0163 | -1.69 | C16H12SO8 | 283.0591, 240.0458 | ＋ | ＋ | - | ＋ | - | ＋ |
| C95 | Physcion-*O*-SO3 | 22.90 | 363.0159 | -2.79 | C16H12SO8 | 283.0586, 240.0432 | - | ＋ | - | ＋ | - | ＋ |
| C96 | Hydroxyphyscion-*O*-SO3 | 34.37 | 379.0098 | -5.35 | C16H12SO9 | 299.0515 | ＋ | - | ＋ | - | ＋ | - |
| C97 | Hydroxyphyscion-*O*-SO3 | 35.12 | 379.0102 | -4.30 | C16H12SO9 | 299.0529 | - | ＋ | - | ＋ | - | ＋ |
| C98 | Hydroxyphyscion-*O*-SO3 | 28.53 | 379.0097 | -5.62 | C16H12SO9 | 299.0528 | - | ＋ | - | ＋ | - | ＋ |
| C99 | Hydroxyphyscion-*O*-SO3 | 25.83 | 379.0098 | -5.35 | C16H12SO9 | 299.0539 | ＋ | ＋ | - | ＋ | ＋ | ＋ |
| C100 | Hydroxyphyscion-*O*-SO3 | 23.28 | 379.0103 | -4.03 | C16H12SO9 | 299.0529 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C101 | Hydroxyphyscion-*O*-SO3 | 23.57 | 379.0102 | -4.30 | C16H12SO9 | 299.0536 | - | ＋ | - | ＋ | - | ＋ |
| C102 | 6-Methylrhein | 32.63 | 297.0379 | -4.93 | C16H10O6 | 253.0491, 225.0528 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C103 | 6-Methylrhein isomer | 35.98 | 297.0381 | -4.26 | C16H10O6 | 253.0452, 225.0511 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C104 | Chrysophanol | 28.16 | 253.0494 | -0.54 | C15H10O4 | 225.053 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C105 | Chrysophanol isomer | 20.36 | 253.0497 | 0.65 | C15H10O4 | 225.0560 | - | ＋ | - | ＋ | - | ＋ |
| C106 | Chrysophanol isomer | 21.09 | 253.0473 | -8.83 | C15H10O4 | 225.0526 | ＋ | ＋ | ＋ | ＋ | - | ＋ |
| C107 | Chrysophanol isomer | 23.99 | 253.0503 | 3.02 | C15H10O4 | 225.0549 | - | ＋ | - | ＋ | - | ＋ |
| C108 | Chrysophanol isomer | 25.31 | 253.0473 | -8.83 | C15H10O4 | 225.0524 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C109 | Chrysophanol isomer | 27.10 | 253.0471 | -9.62 | C15H10O4 | 225.0525 | ＋ | ＋ | ＋ | - | ＋ | - |
| C110 | Chrysophanol isomer | 27.43 | 253.0477 | -7.25 | C15H10O4 | 225.0528 | ＋ | ＋ | ＋ | - | ＋ | - |
| C111 | Chrysophanol isomer | 32.63 | 253.0491 | -1.72 | C15H10O4 | 225.0520 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C112 | Chrysophanol isomer | 35.98 | 253.0468 | -10.81 | C15H10O4 | 225.0505 | ＋ | - | ＋ | - | ＋ | - |
| C113 | Chrysophanol isomer | 36.95 | 253.0498 | 1.05 | C15H10O4 | 225.0534 | - | ＋ | - | ＋ | - | ＋ |
| C114 | Chrysophanol isomer | 38.18 | 253.0497 | 0.65 | C15H10O4 | 225.0538 | - | ＋ | - | ＋ | - | ＋ |
| C115 | Chrysophanol-*O*-GluA | 27.17 | 429.0795 | -4.95 | C21H18O10 | 253.0472, 225.0528 | ＋ | ＋ | ＋ | - | ＋ | - |
| C116 | Chrysophanol-*O*-GluA | 27.51 | 429.0786 | -7.05 | C21H18O10 | 253.0454, 225.0545 | ＋ | ＋ | ＋ | - | ＋ | - |
| C117 | Chrysophanol-*O*-SO3 | 20.11 | 333.0056 | -2.25 | C15H10SO7 | 253.0489, 225.0581 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C118 | Chrysophanol-*O*-SO3 | 21.00 | 333.0087 | 7.06 | C15H10SO7 | 253.0501, 225.0544 | - | ＋ | - | ＋ | - | ＋ |
| C119 | Chrysophanol-*O*-SO3 | 28.16 | 333.0070 | 1.95 | C15H10SO7 | 253.0475, 225.0537 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C120 | Methylate-Chrysophanol | 31.67 | 267.0640 | -4.44 | C16H12O4 | 225.0515 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C121 | Methylate-Chrysophanol | 36.18 | 267.0645 | -2.57 | C16H12O4 | 239.0671 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C122 | Dihydrodeoxygenate- Chrysophanol-*O*-GluA | 20.02 | 417.1189 | 2.14 | C21H22O9 | 241.0839, 135.0453, 121.0294 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C123 | Chrysazin | 21.61 | 239.0316 | -9.56 | C14H8O4 | 211.0367, 183.0429 | ＋ | ＋ | ＋ | - | ＋ | ＋ |
| C124 | Chrysazin isomer or Alizarin isomer | 23.56 | 239.0319 | -8.31 | C14H8O4 | 211.0371, 183.0447 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C125 | Alizarin | 35.98 | 239.0326 | -5.38 | C14H8O4 | 211.0367, 183.0439 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C126 | Emodin Anthrone or its isomer | 20.49 | 255.0629 | -8.96 | C15H12O4 | 213.0542, 145.0655 | ＋ | - | ＋ | - | ＋ | - |
| C127 | Emodin Anthrone or its isomer | 21.00 | 255.0627 | -9.74 | C15H12O4 | 213.0536, 145.0674 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C128 | Emodin Anthrone or its isomer | 23.66 | 255.0657 | 2.02 | C15H12O4 | 213.0554, 145.0668 | - | ＋ | - | ＋ | - | ＋ |
| C129 | Emodin Anthrone or its isomer | 31.21 | 255.0651 | -0.34 | C15H12O4 | 213.0527, 145.0661 | - | ＋ | - | ＋ | - | ＋ |
| C130 | Torachrysone or its isomer | 24.92 | 245.0792 | -6.67 | C14H14O4 | 230.0562, 215.0337, 159.0440 | ＋ | ＋ | ＋ | - | ＋ | + |
| C131 | Torachrysone or its isomer | 27.03 | 245.0802 | -2.59 | C14H14O4 | 230.0558, 215.0329, 159.0441 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C132 | Torachrysone or its isomer | 35.58 | 245.0809 | 0.26 | C14H14O4 | 230.0558, 215.0328, 159.0434 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C133 | Torachrysone or its isomer | 36.66 | 245.0796 | -5.04 | C14H14O4 | 230.0569, 215.0325, 159.0439 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C134 | Carbonylate-Torachrysone | 22.95 | 259.0594 | -2.70 | C14H12O5 | 231.0643, 216.0398, 188.0473, 159.0428 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C135 | Carbonylate-Torachrysone | 27.64 | 259.0591 | -3.86 | C14H12O5 | 215.0681, 173.0585 | ＋ | ＋ | - | - | - | ＋ |
| C136 | Demethylate-Torachrysone-*O*-GluA | 13.76 | 407.0954 | -4.60 | C19H20O10 | 231.0640 | ＋ | ＋ | ＋ | - | ＋ | - |
| C137 | Demethylate-Torachrysone-*O*-GluA | 22.46 | 407.0947 | -6.32 | C19H20O10 | 231.0644 | ＋ | - | - | - | - | - |
| C138 | Hydroxytorachrysone-*O*-SO3 | 23.50 | 341.0338 | 3.62 | C14H14SO8 | 261.0721, 246.0487, 175.0370 | ＋ | - | ＋ | - | ＋ | - |
| C139 | Hydroxytorachrysone-*O*-SO3 | 25.31 | 341.0307 | -5.47 | C14H14SO8 | 261.0728, 246.0496, 231.0275, 175.0398 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C140 | Hydroxytorachrysone | 25.31 | 261.0737 | -7.85 | C14H14O5 | 246.0496, 231.0280, 175.0386 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C141 | Methylate-Hydroxytorachrysone | 17.44 | 275.0920 | 2.18 | C15H16O5 | 231.0671, 189.0565 | - | ＋ | - | ＋ | - | ＋ |
| C142 | Methylate-Hydroxytorachrysone | 19.33 | 275.0914 | 0.00 | C15H16O5 | 231.0646, 189.0551 | - | ＋ | - | ＋ | - | ＋ |
| C143 | Methylate-Hydroxytorachrysone | 20.67 | 275.0917 | 1.09 | C15H16O5 | 231.0683, 189.0558 | - | ＋ | - | ＋ | - | ＋ |
| C144 | Methylate-Hydroxytorachrysone | 24.58 | 275.0930 | 5.82 | C15H16O5 | 231.1005 | ＋ | ＋ | ＋ | ＋ | ＋ | - |
| C145 | Methylate-Hydroxytorachrysone | 30.75 | 275.0905 | -3.27 | C15H16O5 | 231.0999 | ＋ | - | ＋ | - | ＋ | - |
| C146 | Torachrysone-*O*-GluA | 24.92 | 421.1097 | -7.65 | C20H22O10 | 245.0788, 230.0553, 215.0334, 159.0449 | ＋ | ＋ | ＋ | - | ＋ | - |
| C147 | Torachrysone-*O*-SO3 | 27.03 | 325.0352 | -7.54 | C14H14SO7 | 245.0786, 230.0546, 215.0326, 159.0440 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C148 | Demethylate-Torachrysone | 16.58 | 231.0648 | -1.67 | C13H12O4 | 145.0603 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C149 | Demethylate-Torachrysone | 21.09 | 231.0633 | -8.16 | C13H12O4 | 145.0653 | ＋ | - | - | - | - | - |
| C150 | Demethylate-Torachrysone | 22.67 | 231.0635 | -7.29 | C13H12O4 | 145.0650 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C151 | Demethylate-Torachrysone | 24.04 | 231.0634 | -7.73 | C13H12O4 | 145.0629 | ＋ | ＋ | - | ＋ | - | ＋ |
| C152 | Caffeic acid | 15.23 | 179.0352 | 7.34 | C9H8O4 | 135.0453, 107.0500 | - | - | - | ＋ | - | ＋ |
| C153 | Caffeic acid isomer | 12.83 | 179.0352 | 7.34 | C9H8O4 | 135.0443, 107.0493 | - | ＋ | - | ＋ | - | ＋ |
| C154 | Caffeic acid isomer | 13.99 | 179.0342 | 1.76 | C9H8O4 | 135.0454, 107.0479 | ＋ | - | ＋ | - | ＋ | - |
| C155 | Caffeic acid isomer | 14.28 | 179.0349 | 5.67 | C9H8O4 | 135.0462, 107.0523 | - | ＋ | - | ＋ | - | ＋ |
| C156 | Caffeic acid isomer | 16.24 | 179.0348 | 5.11 | C9H8O4 | 135.0457, 107.0501 | - | ＋ | - | ＋ | - | ＋ |
| C157 | Caffeic acid isomer | 16.79 | 179.0350 | 6.23 | C9H8O4 | 135.0451, 107.0497 | - | ＋ | - | ＋ | - | ＋ |
| C158 | Methylate-Caffeic acid | 14.30 | 193.0497 | 0.85 | C10H10O4 | 149.0595 | ＋ | ＋ | ＋ | ＋ | ＋ | - |
| C159 | Methylate-Caffeic acid | 16.48 | 193.0502 | 3.44 | C10H10O4 | 149.0597 | - | ＋ | - | ＋ | - | ＋ |
| C160 | Methylate-Caffeic acid | 17.49 | 193.0505 | 5.00 | C10H10O4 | 149.0594 | - | ＋ | - | ＋ | - | ＋ |
| C161 | Methylate-Caffeic acid | 18.56 | 193.0502 | 3.44 | C10H10O4 | 149.0588 | - | ＋ | - | ＋ | - | ＋ |
| C162 | Methylate-Caffeic acid | 20.97 | 193.0502 | 3.44 | C10H10O4 | 149.0595 | - | ＋ | - | ＋ | - | ＋ |
| C163 | Methylate-Caffeic acid-*O*-SO3 | 14.30 | 273.0074 | 3.85 | C10H10SO7 | 193.0490, 149.0588 | ＋ | ＋ | ＋ | ＋ | ＋ | - |
| C164 | Methylate-Caffeic acid-*O*-SO3 | 15.80 | 273.0068 | 1.65 | C10H10SO7 | 193.0500, 149.0621 | - | ＋ | - | ＋ | - | ＋ |
| C165 | Methylate-Caffeic acid-*O*-SO3 | 16.48 | 273.0068 | 1.65 | C10H10SO7 | 193.0507, 149.0558 | - | ＋ | - | ＋ | - | ＋ |
| C166 | Methylate-Caffeic acid-*O*-SO3 | 17.49 | 273.0068 | 1.65 | C10H10SO7 | 193.0505, 149.0606 | - | ＋ | - | ＋ | - | ＋ |
| C167 | Caffeic acid-*O*-SO3 | 13.99 | 258.9891 | -6.18 | C9H8O7S | 179.0344, 135.0443, 107.0508 | ＋ | - | ＋ | - | ＋ | - |
| C168 | Dehydrogenate-Caffeic acid | 14.79 | 177.0185 | 1.50 | C9H6O4 | 133.0293, 105.0349 | ＋ | ＋ | ＋ | - | ＋ | - |
| C169 | Dehydrogenate-Caffeic acid | 19.70 | 177.0190 | 4.32 | C9H6O4 | 133.0291, 105.0343 | - | ＋ | - | ＋ | - | ＋ |
| C170 | Cinnamic acid | 17.30 | 147.0445 | 3.02 | C9H8O2 | 103.0563 | ＋ | ＋ | ＋ | ＋ | ＋ | - |
| C171 | Cinnamic acid isomer | 7.73 | 147.0453 | 8.46 | C9H8O2 | 103.0556 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C172 | Cinnamic acid isomer | 24.19 | 147.0435 | -3.78 | C9H8O2 | 103.0556 | ＋ | ＋ | ＋ | ＋ | ＋ | - |
| C173 | Hydroxycinnamic acid | 5.11 | 163.0395 | 3.25 | C9H8O3 | 119.0500 | ＋ | ＋ | ＋ | - | ＋ | - |
| C174 | Hydroxycinnamic acid | 13.99 | 163.0397 | 4.47 | C9H8O3 | 119.0499 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C175 | Hydroxycinnamic acid | 14.82 | 163.0398 | 5.09 | C9H8O3 | 119.0509 | - | - | - | - | - | ＋ |
| C176 | Hydroxycinnamic acid | 17.90 | 163.0396 | 3.86 | C9H8O3 | 119.0505 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C177 | Hydrate-Hydroxycinnamic acid | 11.72 | 181.0498 | 1.46 | C9H10O4 | 163.0399, 119.0503 | ＋ | ＋ | ＋ | - | ＋ | - |
| C178 | Hydroxycinnamic acid-*O*-SO3 | 13.08 | 242.9968 | 4.18 | C9H8SO6 | 163.0402, 119.0495 | - | - | - | ＋ | - | ＋ |
| C179 | Hydroxycinnamic acid-*O*-SO3 | 13.99 | 242.9969 | 4.59 | C9H8SO6 | 163.0393, 119.0502 | ＋ | - | ＋ | - | ＋ | ＋ |
| C180 | Malic acid | 3.53 | 133.0121 | -7.89 | C4H6O5 | 115.0012 | ＋ | - | ＋ | - | ＋ | - |
| C181 | Resveratrol 4'-*O*-*β*-D-glucopyranoside | 24.70 | 389.1239 | 2.07 | C20H22O8 | 227.0680 | ＋ | - | - | - | - | - |
| C182 | Aloesol | 15.21 | 233.0803 | -2.30 | C13H14O4 | 189.0565, 149.0237, 105.0352 | ＋ | ＋ | ＋ | - | ＋ | - |
| C183 | Aloesol | 18.33 | 233.0798 | -4.44 | C13H14O4 | 189.0540, 149.0222, 105.0342 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C184 | Aloesol | 21.82 | 233.0794 | -6.16 | C13H14O4 | 189.0548, 149.0230, 105.0345 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C185 | Coumalic acid isomer | 5.11 | 163.0395 | 3.25 | C9H8O3 | 119.0500 | ＋ | ＋ | ＋ | - | ＋ | - |
| C186 | Coumalic acid isomer | 13.99 | 163.0397 | 4.47 | C9H8O3 | 119.0502 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |
| C187 | Coumalic acid | 17.90 | 163.0396 | 3.86 | C9H8O3 | 119.0505 | ＋ | ＋ | ＋ | ＋ | ＋ | - |
| C188 | Methoxy-galloylglucose | 6.59 | 345.0817 | 0.22 | C14H18O10 | 183.0285, 168.0050 | - | ＋ | - | ＋ | - | - |
| C189 | Methoxy-galloylglucose | 7.51 | 345.0830 | 3.99 | C14H18O10 | 183.0277, 168.0037 | - | ＋ | - | ＋ | - | - |
| C190 | Methoxy-galloylglucose | 8.02 | 345.0824 | 2.25 | C14H18O10 | 183.0308, 168.0080 | - | ＋ | - | ＋ | - | - |
| C191 | Methoxy-galloylglucose | 9.01 | 345.0824 | 2.25 | C14H18O10 | 183.0287, 168.0052 | ＋ | - | - | - | - | - |
| C192 | Methoxy-galloylglucose | 11.19 | 345.0801 | -4.41 | C14H18O10 | 183.0313, 168.0059 | - | ＋ | - | ＋ | - | ＋ |
| C193 | Galloylglucose | 3.76 | 331.0644 | -4.75 | C13H16O10 | 211.0213, 169.0128, 151.0037, 125.0237 | ＋ | - | ＋ | ＋ | ＋ | - |
| C194 | Galloylglucose | 5.11 | 331.0649 | -3.24 | C13H16O10 | 211.0211, 169.0146, 151.0037, 125.0246 | ＋ | - | - | - | ＋ | - |
| C195 | Galloylglucose | 5.38 | 331.0649 | -3.24 | C13H16O10 | 211.0287, 169.0146, 151.0023, 125.0213 | ＋ | ＋ | - | - | ＋ | - |
| C196 | Galloylglucose | 6.23 | 331.0653 | -2.03 | C13H16O10 | 211.0231, 169.0140, 151.0004, 125.0247 | ＋ | ＋ | ＋ | ＋ | ＋ | ＋ |

Note: P: plasma; U: urine.