Supplementary Material

# Supplementary Figures and Tables

## Supplementary Figures



**Supplementary Figure 1.** Total ion chromatograms of Kouyanqing Granule (KYQG) in positive mode (A) and negative mode (B).

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**Supplementary Figure 2.** Total ion chromatograms of standards in positive mode (A) and negative mode (B).

## Supplementary Tables

**Supplementary Table 1.** The mass spectrum data of standards. The losses are: Glc = glucose moiety.

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| --- | --- | --- | --- | --- | --- | --- | --- |
| No. | RT(min) | Formula | [M+H]+(Error, ppm) | [M–H]–(Error, ppm) | MS/MS fragments(Positive mode) | MS/MS fragments(Negative mode) | Standard |
| 1 | 5.25 | C6H14N2O2 | 147.1128（+0.7） |  | 130.0868 [M+H–NH3]+,84.0828 [M+H–NH3–HCOOH]+,67.0573 [M+H–2NH3–HCOOH]+ |  | Lysine |
| 2 | 5.55 | C6H14N4O2 | 175.1188（–0.9） | 173.1057（+5.1） | 158.0921 [M+H–NH3]+,130.0976 [M+H–NH3–CO]+,116.0706 [M+H–CN3H5]+70.0676 [M+H–CN3H5–HCOOH]+,60.0586 | 156.0766 [M–H–NH3]–,131.0828 [M–H–C3H6]– | Arginine |
| 4 | 5.87 | C4H7NO4 |  | 132.0323（+9.1） |  | 115.0045 [M–H–NH3]–,88.0410 [M–H–CO2]–,71.0151 [M–H– CO2–NH3]– | Aspartic acid |
| 6 | 6.18 | C6H13N3O3 | 176.1031（+0.8） |  | 159.0766 [M+H–NH3]+,113.0718 [M+H–NH3–HCOOH]+,70.0677 [M+H–NH3–CO2–CH3NO]+ |  | Citrulline |
| 18 | 10.71 | C7H4O6 | 185.0080（–0.2） | 182.9946（+6） | 141.0182 [M+H–CO2]+,97.0294 [M+H–2CO2]+,71.0151 [M+H–2CO2–C2H2]+ | 139.0043 [M–H–CO2]–,68.9998 [M–H–C4H2O4]–,67.0211 [M–H–2CO2–CO]– | Chelidonic acid |
| 26 | 17.11 | C9H11NO2 | 166.0861（–0.8） | 164.0730（+7.7） | 120.0813 [M+H–HCOOH]+,103.0552 [M+H–HCOOH–NH3]+ | 147.0454 [M–H–NH3]–,103.0555 [M–H–NH3–CO2]–,72.0111 | Phenylalanine |
| 32 | 28.48 | C16H18O9 | 355.1027（+1） | 353.0877（–0.4） | 163.0385 [M+H–C7H12O6]+,145.0281 [M+H–C7H12O6–H2O]+,117.0337 [M+H–C7H12O6–H2O–CO]+,89.0392 [M+H–C7H12O6–H2O–2CO]+ | 191.0567 [M–H–C9H6O3]– | Chlorogenic acid |
| 35 | 35.26 | C9H8O4 | 181.0409（–0.7） | 179.0360（+1.9） | 163.0387 [M+H–H2O]+,135.0439 [M+H–HCOOH]+,89.398 [M+H–H2O–CO–HCOOH]+ | 135.0455 [M–H–CO2]– | Caffeic acid |
| 44 | 48.8 | C21H22O9 | 419.1334（–0.7） | 417.1185（–0.1.4） | 257.0808 [M+H–Glc]+,137.0231 [M+H–C14H18O6]+ | 255.0665 [M–H–Glc]–,135.0096 [M–H–Glc–RAD]–,119.0512 | Liquiritin |
| 45 | 49.6 | C21H20O12 | 465.1022（–0.6） | 463.0858（–3.7） | 303.0490 [M+H–Glc]+ | 301.0343 [M–H–Glc]–,271.0246 [M–Glc–CH2O]–,255.0301 [M–H–Glc–O–CH2O]–,151.0040 [M–H–Glc–RDA]– | Isoquercitrin |
| 51 | 57.26 | C36H48O19 | 807.2675（–0.9） | 783.2697（–2.5） | 807.2675 [M+Na]+ | 607.2250 [M–H–C6H11O4–CHO]–193.0506 [M–H–C26H38O15]–,175.0396 [M–H–C26H38O15–H2O]– | Angoroside C |
| 56 | 48.8 | C21H22O9 | 419.1334（–0.7） | 417.1185（–1.4） | 257.0808 [M+H–Glc]+,137.0231 [M+H–Glc–C8H6O]+ | 255.0665 [M–H–Glc]–,135.0096,119.0512 [M–H–Glc–C8H6O–H2O]–,92.0260 [M–H–Glc–C9H7O3]– | Isoliquiritoside |
| 57 | 74.11 | C24H30O11 | 517.1675（–1.0） | 493.1685（–6.1） | 369.1170,203.0533 | 345.1167 [M–H–C9H7O2]–,147.0451 [M–H–C15H22O9]–,165.0553,103.0558 | Harpagoside |
| 61 | 75.42 | C65H106O32 |  | 1397.6516（–1.1） |  | 1073.5549 [M–H–2Glc]–,744.3308 | Macranthoidin B |
| 62 | 76.91 | C15H10O6 | 287.0553（+0.8） | 285.0404（–0.1） | 153.0181 [M+H–C8H6O2]+ | 175.00403 [M–H–C6H6O2]–,133.0305 [M–H–C7H4O4]– | Luteolin |
| 66 | 78.14 | C15H10O7 |  | 301.0305（–0.7） |  | 178.9993 [M–H–C7H6O2]–,151.0044 [M–H–C8H6O3]– | Quercetin |
| 71 | 91.91 | C16H12O6 | 301.0708（+0.4） | 299.0563（–0.6） | 286.0477 [M+H–CH3]+,258.0530 [M+H–CH3–CO]+,119.0487,153.0189 | 284.0325 [M–H–CH3]–,256.0388 [M–H–CH3–CO]–,227.0363 [M–H–CH3–CO–CHO]– | Diosmetin |
| 76 | 102.9 | C16H12O4 | 269.0810（+0.5） | 267.0660（–1.2） | 253.0551 [M+H–CH3]+,197.0600 [M–CH3 –CO–CO]+,181.0649 [M–OCH3 –CO–CO]+ | 252.0427 [M–H–CH3]–,223.0407 [M–H–CH3–CHO]–,195.0457 [M–H–CH3–CHO–CO]–,132.0232 [M–H–C7H7O– CO]–,91.0210 [M–H–C9H8O– CO–OH]– | Formononetin |