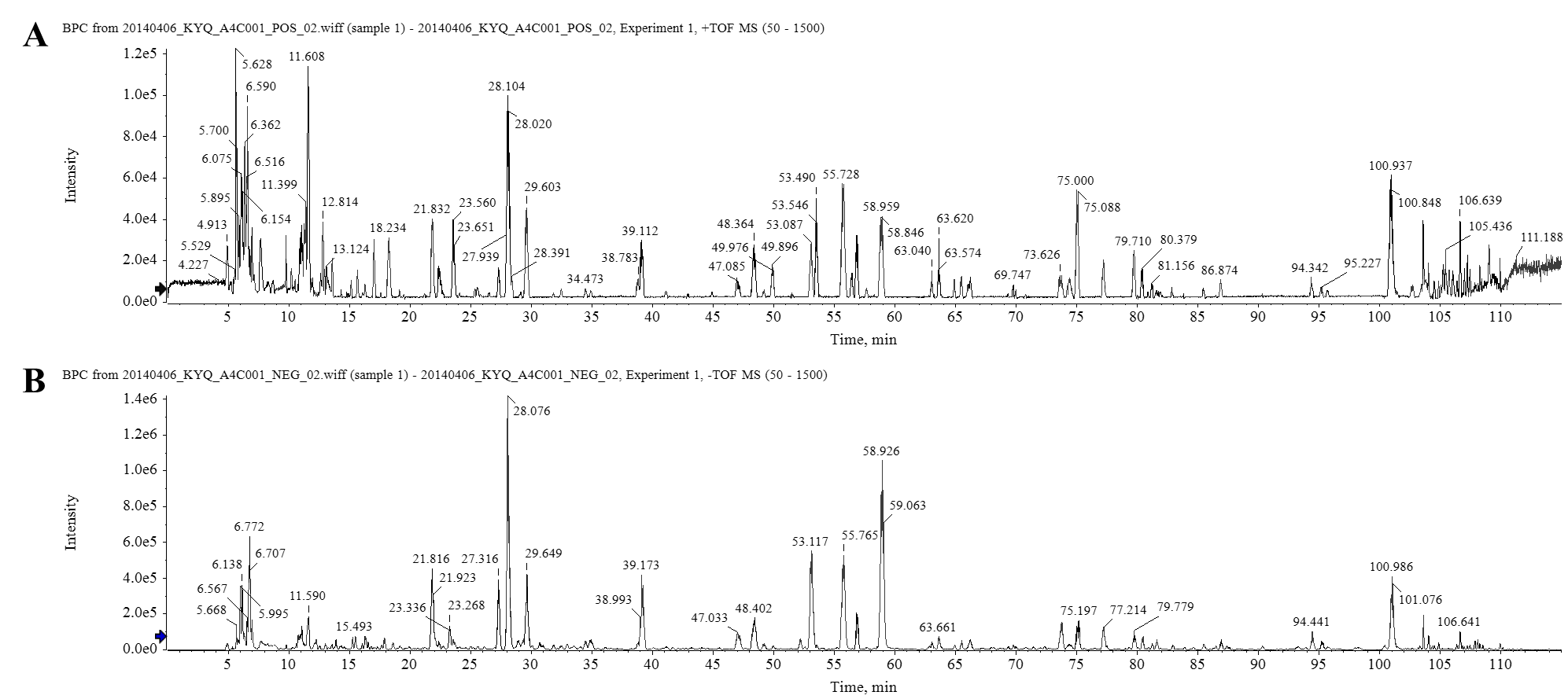
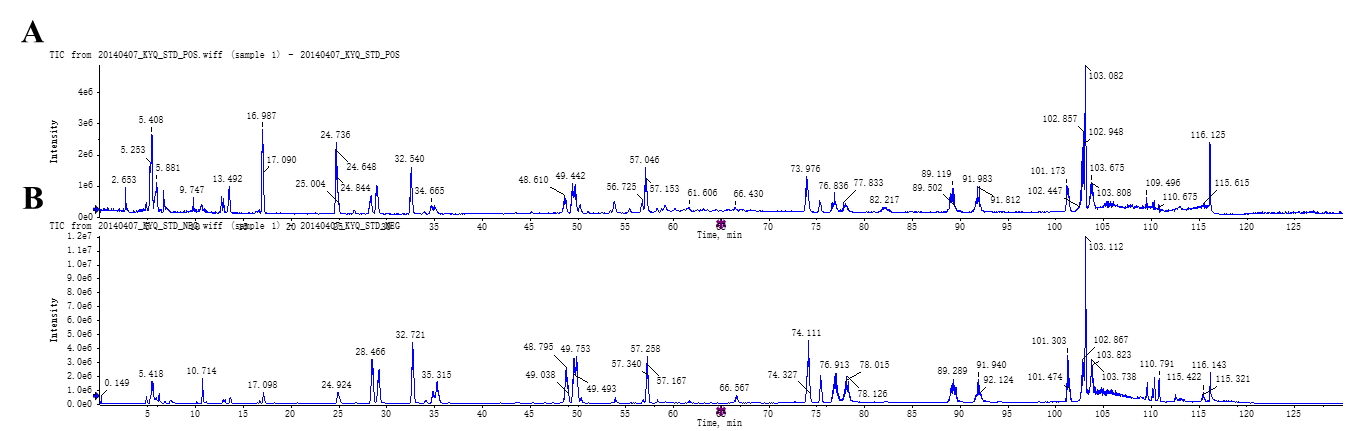
Supplementary Material

# 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.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |