

**Table S1.** Retention time、 maximum absorption UV wavelength and the MS data of compound 1, 2, 3, 5, 7, 9, 11, and 12 selected from PLR.

| Peak | TR   | UV<br>(nm) | Identification                               | Formula   | Negative ion(m/z)  |                        |                | Positive ion(m/z)  |                             |                |          |
|------|------|------------|--|---|--|------------------------|----------------|--|-----------------------------|----------------|----------|
|      |      |            |  |   | Proposal ions  | MS/MS                  | Error<br>(ppm) | Proposal ions  | MS/MS                       | Error<br>(ppm) |          |
| 1    | 25.7 | 248        | Puerarin                                     | C <sub>21</sub> H <sub>20</sub> O <sub>9</sub>  | [M-H] <sup>-</sup>   | 415.1034               | 0.13           | [M+H] <sup>+</sup>   | 417.1180                    | -1.42          |          |
|      |      | 305        |  |   | [M- C <sub>4</sub> H <sub>8</sub> O <sub>4</sub> -H] <sup>-</sup>                  | 295.0605               |                | [M+H-2H <sub>2</sub> O- C <sub>4</sub> H <sub>4</sub> O <sub>2</sub> ] <sup>+</sup>                  | 297.0765                    |                |          |
|      |      |            |  |   | [M- C <sub>4</sub> H <sub>8</sub> O <sub>4</sub> -H <sub>2</sub> O-H] <sup>-</sup> | 277.0488               |                | [M+H-2H <sub>2</sub> O-CH <sub>2</sub> O-C <sub>4</sub> H <sub>4</sub> O <sub>2</sub> ] <sup>+</sup> | 267.0652                    |                |          |
| 2    | 32.6 | 247        | Mirificin                                    | C <sub>26</sub> H <sub>28</sub> O <sub>13</sub> | [M-H] <sup>-</sup>   | 547.1451               | 1.12           | [M+H] <sup>+</sup>   | 549.1601                    | 0.31           |          |
|      |      | 306        |  |   | [M-api- C <sub>4</sub> H <sub>7</sub> O <sub>3</sub> -H] <sup>-</sup>              | 295.0603               |                | [M+H-api] <sup>+</sup>   | 417.1138                    |                |          |
|      |      |            |  |   | [M-api- C <sub>4</sub> H <sub>7</sub> O <sub>3</sub> -CO-H] <sup>-</sup>           | 267.0653               |                | [M+H-api-2H <sub>2</sub> O-CH <sub>2</sub> O] <sup>+</sup>   | 351.0980                    |                |          |
| 3    | 39.3 | 248        | Daidzin                                      | C <sub>21</sub> H <sub>20</sub> O <sub>9</sub>  | [M+HCOO-H] <sup>-</sup>  | 461.1082               | 1.77           | [M+H] <sup>+</sup>   | 417.1182                    | -0.46          |          |
|      |      |            |  |   |  | [M-H] <sup>-</sup>     |                | 415.1007   | [M+H-glc] <sup>+</sup>      |                | 255.0655 |
|      |      |            |  |   |  | [M-glc-H] <sup>-</sup> |                | 253.0491   |                             |                |          |
| 5    | 47.5 | 206        | Genistin                                     | C <sub>21</sub> H <sub>20</sub> O <sub>10</sub> | [M+HCOO-H] <sup>-</sup>  | 477.1035               | 0.81           | [M+H] <sup>+</sup>   | 433.1137                    | -1.8           |          |
|      |      | 263        |  |   | [M-glc-H] <sup>-</sup>   | 269.0331               |                | [M+H-glc] <sup>+</sup>   | 271.0618                    |                |          |
| 7    | 56.2 | 208        | Genistein-8-C-<br>apiosyl(1-6)-<br>glucoside | C <sub>26</sub> H <sub>28</sub> O <sub>14</sub> | [M-H] <sup>-</sup>   | 563.1401               | 0.94           | [M+H] <sup>+</sup>   | 565.1544                    | 1.39           |          |
|      |      | 244        |  |   | [M-api- C <sub>4</sub> H <sub>7</sub> O <sub>3</sub> -H] <sup>-</sup>              | 310.9359               |                |  |                             |                |          |
|      |      |            |  |   | [M-api- C <sub>4</sub> H <sub>7</sub> O <sub>3</sub> -CO-H] <sup>-</sup>           | 283.9540               |                |  |                             |                |          |
| 9    | 62.6 | 249        | Malonyl-<br>Daidzin                          | C <sub>24</sub> H <sub>22</sub> O <sub>12</sub> | [M-H] <sup>-</sup>   | 501.1026               | 2.49           | [M+H] <sup>+</sup>   | 503.1183                    | 0.20           |          |
| 11   | 68.7 | 242        | Sophoroside A                                | C <sub>24</sub> H <sub>26</sub> O <sub>10</sub> | [M-H] <sup>-</sup>   | 473.1458               | -1.01          | [M+H] <sup>+</sup>   | 475.1594                    | 1.00           |          |
|      |      | 264        |  |   |  |                        |                | [M+H-glc] <sup>+</sup>   | 313.1073                    |                |          |
|      |      |            |  |   |  |                        |                | [M+H-glc-CO <sub>2</sub> ] <sup>+</sup>  | 267.2674                    |                |          |
| 12   | 71.0 | 261        | Malonyl-<br>Genistin                         | C <sub>24</sub> H <sub>22</sub> O <sub>13</sub> | [M-H] <sup>-</sup>   | 517.1013               | -4.89          | [M+H] <sup>+</sup>   | 519.1141                    | -1.51          |          |
|      |      |            |  |   |  |                        |                |  | [M+H-(mal)glc] <sup>+</sup> |                | 271.1492 |