

**Table S1.** Non-targeted analysis of extracts of *L. gmelinii* root in (+)ESI mode using LC-QToF.

| #  | RT (min)  | Compound Name   | Formula   | Mass     | [M+H] <sup>+</sup>     | Fragment Ions        |
|----|-----------|---|---|----------|------------------------|----------------------|
| 1  | 11.5      | Myricetin 7-rhamnoside/Myricetin 3-O- $\alpha$ -L-rhamnopyranoside (Myricitrin)                   | C <sub>21</sub> H <sub>20</sub> O <sub>12</sub> | 464.0955 | 465.1025<br>(465.1028) | 319.0439             |
| 2  | 11.6      |   |   |          |                        |                      |
| 3  | 9.93      | Myricetin 3-galactoside (Gmelinoside I)/<br>Myricetin 3- $\beta$ -D-sorbose/Myricetin 3-glucoside | C <sub>21</sub> H <sub>20</sub> O <sub>13</sub> | 480.0904 | 481.0975<br>(481.0977) | 319.0436             |
| 4  | 10.26     |   |   |          |                        |                      |
| 5  | 10.45     |   |   |          |                        |                      |
| 6  | 12.41     |   |   |          |                        |                      |
| 7  | 14.6      | 2',4',5,5',7-Pentahydroxyflavonol/5'-Hydroxymorin   | C <sub>15</sub> H <sub>10</sub> O <sub>8</sub>  | 318.0376 | 319.0439<br>(319.0448) | -                    |
| 8  | 9.63      | Myricetin 7-(6"-galloylglucoside)   | C <sub>28</sub> H <sub>24</sub> O <sub>17</sub> | 632.1013 | 633.1081<br>(633.1086) | 319.0431<br>153.0131 |
| 9  | 10.8      | Myricetin 3-xyloside  | C <sub>20</sub> H <sub>18</sub> O <sub>12</sub> | 450.0798 | 451.0869<br>(451.0871) | 319.0433             |
| 10 | 11.3      |   |   |          |                        |                      |
| 11 | 12.1      | Laricitrin 7-glucoside  | C <sub>22</sub> H <sub>22</sub> O <sub>13</sub> | 494.106  | 495.1121<br>(495.1133) |                      |
| 12 | 11.8/12.2 | Quercetin glucoside   | C <sub>21</sub> H <sub>19</sub> O <sub>12</sub> | 464.0955 | 465.1021<br>(465.1028) | 303.0509             |
| 13 | 10.9      | Quercetin 3-(2"-galloylgalactoside  | C <sub>28</sub> H <sub>24</sub> O <sub>16</sub> | 616.1064 | 617.1131<br>(617.1137) | 303.0441             |
| 14 | 12.3      | Myricetin-3-O-[3,4,5-Trihydroxybenzoyl-( $\rightarrow$ 2)- $\alpha$ -L-arabinopyranoside]         | C <sub>27</sub> H <sub>22</sub> O <sub>16</sub> | 602.0908 | 603.0975<br>(603.0981) | 319.0429<br>153.0164 |
| 15 | 9.2       | Epigallocatechin gallate/Gallo epicatechin gallate  | C <sub>22</sub> H <sub>18</sub> O <sub>11</sub> | 458.0849 | 459.0927<br>(459.0922) | 139.0396             |
| 16 | 8.8       | Epicatechin/Catechin  | C <sub>15</sub> H <sub>14</sub> O <sub>6</sub>  | 290.079  | 291.0857<br>(291.0863) | 139.0391             |
| 17 | 4.07      | Gallocatechin/Epigallocatechin/<br>3,5,7,3',4',6'-hexahydroxyflavan                               | C <sub>15</sub> H <sub>14</sub> O <sub>7</sub>  | 306.074  | 307.0811<br>(307.0812) | 139.0357             |
| 18 | 4.5       |   |   |          |                        |                      |
| 19 | 5.4       |   |   |          |                        |                      |
| 20 | 6.45      |   |   |          |                        |                      |
| 21 | 3.8       | Phenylalanine   | C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>  | 165.079  | 166.0861<br>(166.0859) | 103.0536<br>77.0385  |
| 22 | 18.5      | Dihydrosyringetin   | C <sub>17</sub> H <sub>15</sub> O <sub>8</sub>  | 346.0689 | 347.0755<br>(347.0761) | -                    |
| 23 | 9.02      | Aromadendrene   | C <sub>15</sub> H <sub>12</sub> O <sub>6</sub>  | 288.0634 | 289.0701<br>(289.0707) | -                    |

|    |       |  |                      |           |                        |                                   |
|----|-------|--|----------------------|-----------|------------------------|-----------------------------------|
| 24 | 3.09  | Gallic Acid  | $C_7H_4O_5$          | 168.0059  | 169.0129<br>(169.0131) | 125.0258                          |
| 25 | 13.4  | Quercitrin   | $C_{21}H_{20}O_{11}$ | 448.1006  | 449.1071<br>(449.1078) | 303.04951                         |
| 26 | 3.9   | (-)-Epigallocatechin-(4 $\beta$ →8)-(-)-3,5,7-3',4',6'-hexahydroxyflavan                               | $C_{30}H_{26}O_{14}$ | 610.1323  | 611.1401<br>(611.1395) | 307.0799<br>139.0351              |
| 27 | 17.5  | Kaempferol   | $C_{15}H_{10}O_6$    | 286.0477  | 287.0545<br>(287.055)  | -                                 |
| 28 | 6.6   | (-)-Epigallocatechin-(4 $\beta$ →8)-(-)-epigallocatechin-3-O-gallate                                   | $C_{37}H_{30}O_{18}$ | 762.1432  | 763.1499<br>(763.1505) | 307.0801,<br>153.0212<br>139.0404 |
| 29 | 15.5  | Limonium A   | $C_{26}H_{19}NO_7$   | 457.1162  | 458.1231<br>(458.1234) | 287.0404                          |
| 30 | 16.79 | Limonium B   | $C_{27}H_{21}NO_7$   | 471.1318  | 472.1385<br>(472.1391) |                                   |
| 31 | 17.1  | Limonium F/H/I/Cannabisin C  | $C_{35}H_{34}N_2O_8$ | 610.2315  | 611.2398<br>(611.2388) |                                   |
| 32 | 17.3  |  |                      |           |                        |                                   |
| 33 | 17.9  |  |                      |           |                        |                                   |
| 34 | 15.77 | Cannabisin B   | $C_{34}H_{32}N_2O_8$ | 596.2159  | 597.2245<br>(597.2231) | 295.0478                          |
| 35 | 15.52 | Cannabisin A   | $C_{34}H_{30}N_2O_8$ | 594.2002  | 595.2071<br>(595.2075) |                                   |
| 36 | 18.6  | Cannabisin D/F   | $C_{36}H_{36}N_2O_8$ | 624.2472  | 625.2535<br>(625.2544) |                                   |
| 37 | 18.8  |  |                      |           |                        |                                   |
| 38 | 20.9  |  |                      |           |                        |                                   |
| 39 | 16.4  | <i>N-trans</i> -feruloyl tyramine  | $C_{18}H_{19}NO_4$   | 313.1314  | 314.1381<br>(314.1381) | 177.0448<br>145.0183<br>117.0241  |
| 40 | 19.3  | Thoreliamide B   | $C_{28}H_{29}NO_8$   | 507.1893  | 508.1956<br>(508.1966) |                                   |
| 41 | 15.65 | 3,3'-Demethyl-heliotropamide   | $C_{34}H_{32}N_2O_8$ | 596.2159  | 597.2223<br>(597.2231) | 295.0460<br>187.0261<br>153.0057  |
| 42 | 5.9   | (+)–gallocatechine–(4 $\alpha$ →8)–[(-)–epigallocatechin]5–(4 $\beta$ →8)–(-)–epigallocatechin gallate | $C_{52}H_{42}O_{25}$ | 1066.2015 | 1067.2088              | 153.0089<br>139.0293              |
| 43 | 8.19  |  |                      |           |                        |                                   |