

## **Supplementary material for:**

### **Glycosides and flavonoids from the extract of *Pueraria thomsonii* Benth leaf alleviates type 2 diabetes in high-fat diet-streptozotocin-induced mice by modulated gut microbiota**

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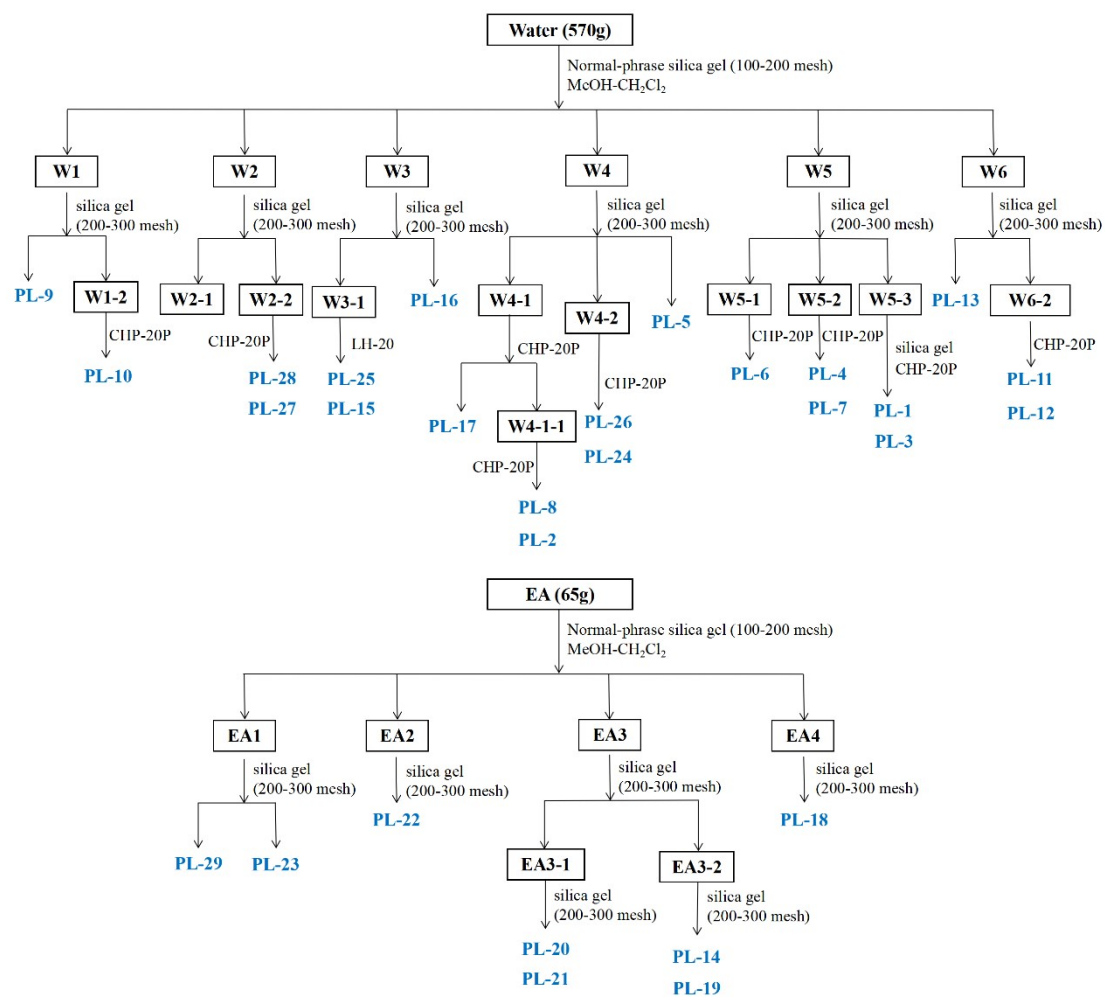


Fig. S1 The separation of water fraction and ethyl acetate fraction.

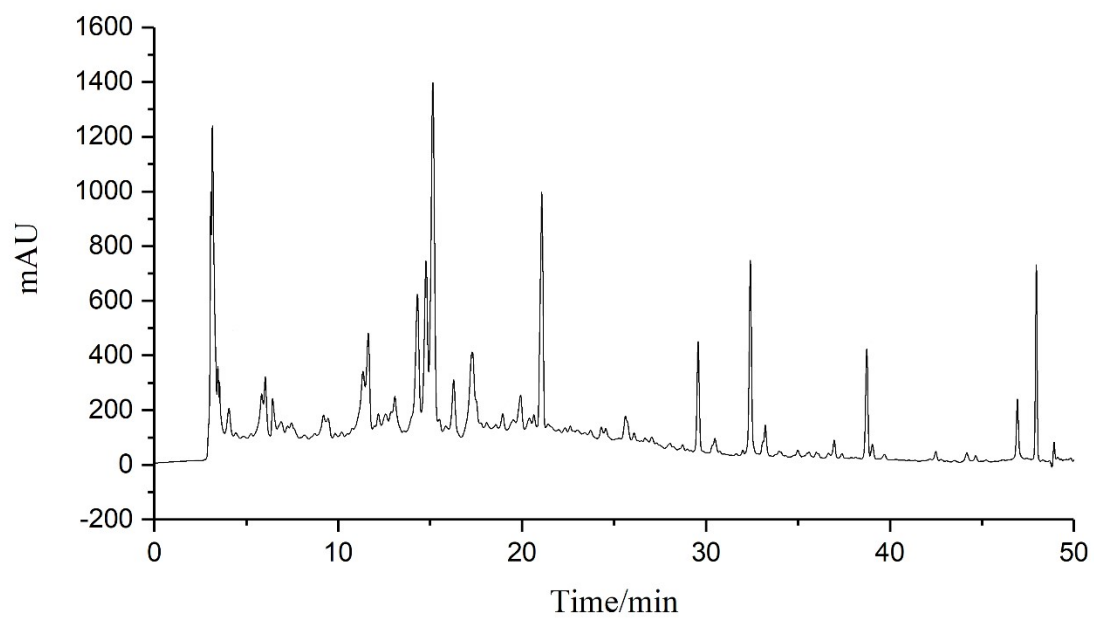


Fig. S2 The HPLC chromatogram of PL sample.

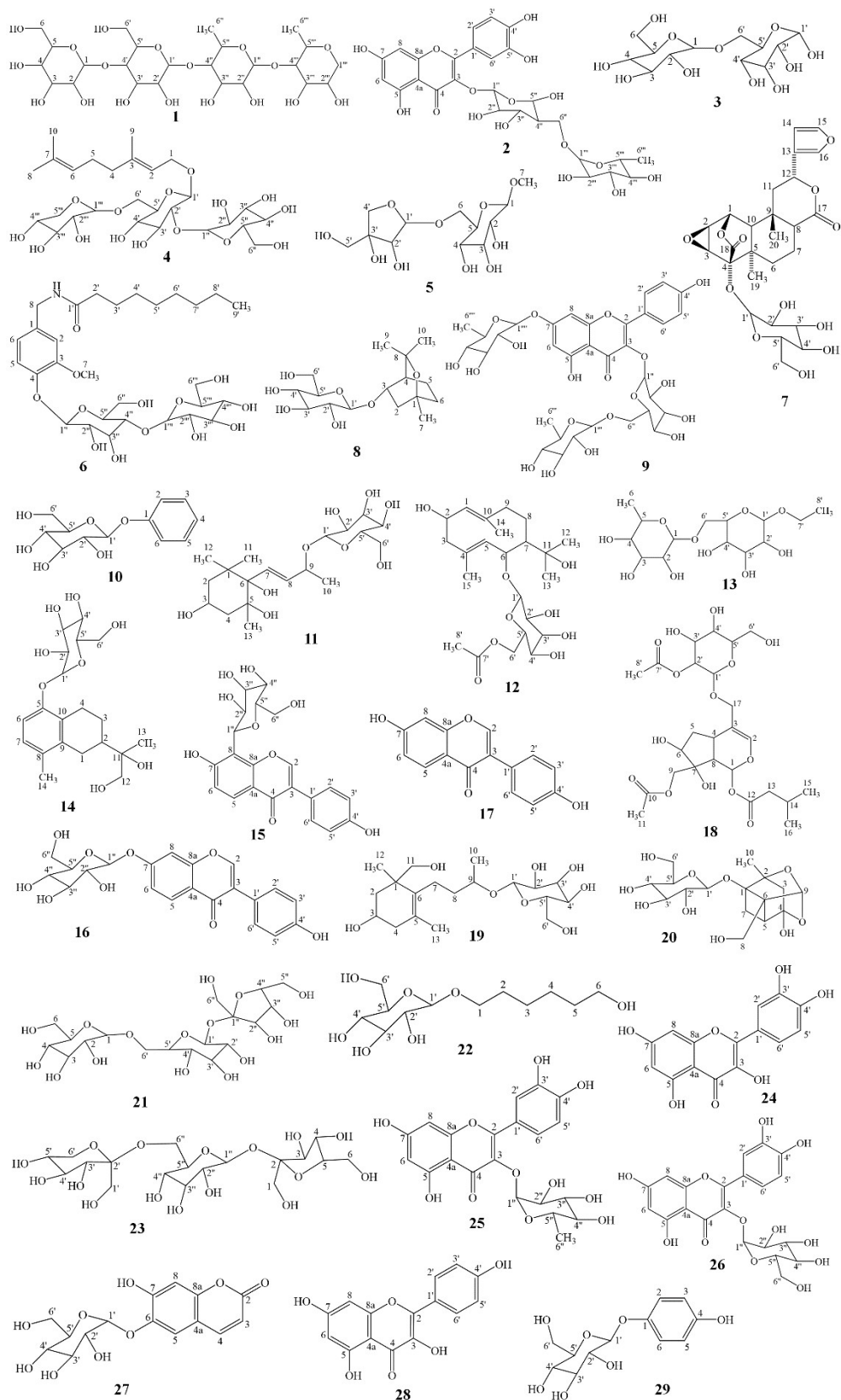


Fig. S3 The chemical structures of glycosides (1, 3-8, 10-14, 18-23, 27, 29) and flavonoids (2, 9, 15-17, 24-26, 28) isolated from the extract of *P. thomsonii* leaf.

Table S1. The quantitation of twenty-nine compounds from the extract of *P. thomsonii* leaf

No.	Calibration curves <sup>a</sup>	R <sup>2</sup>	LOD( $\mu\text{g/mL}$ )	LOQ( $\mu\text{g/mL}$ )	Content(mg/g)
<b>PL-1</b>	$y=0.1538x+141.12$	0.9997	0.10	0.40	46.55
<b>PL-2</b>	$y=14.414x-2841.3$	0.9998	0.05	0.30	0.24
<b>PL-3</b>	$y=14.32x+502.75$	0.9996	0.15	0.50	10.08
<b>PL-4</b>	$y=8.8548x-258.53$	0.9992	0.20	1.00	9.06
<b>PL-5</b>	$y=9.6148x+308.95$	0.9995	0.50	1.50	0.8
<b>PL-6</b>	$y=10.735x+226.54$	0.9992	0.25	1.25	0.46
<b>PL-7</b>	$y=5.0078x+69.557$	0.9989	0.05	0.20	12.55
<b>PL-8</b>	$y=6.6405x-91.606$	0.9999	0.50	2.50	0.79
<b>PL-9</b>	$y=3.7093x+57.2$	0.9997	0.25	1.25	49.28
<b>PL-10</b>	$y=13.374x-74.239$	0.9994	0.15	1.00	10.52
<b>PL-11</b>	$y=9.4538x+702.68$	0.9998	0.20	1.00	11.65
<b>PL-12</b>	$y=6.9002x+111.2$	0.9999	0.05	0.20	6.72
<b>PL-13</b>	$y=4.0568x+750.56$	0.9989	0.15	0.50	3.79
<b>PL-14</b>	$y=3.0804x+230.23$	0.9991	0.25	1.25	10.85
<b>PL-15</b>	$y=16.289x-24.79$	0.9997	0.50	2.50	42.87
<b>PL-16</b>	$y=35.174x-85.82$	0.9991	1.00	2.50	13.65
<b>PL-17</b>	$y=2.11x-26.58$	0.9999	0.05	0.20	10.54
<b>PL-18</b>	$y=2.1727x+91.88$	0.9988	0.05	0.25	12.04
<b>PL-19</b>	$y=4.6759x+199.1$	0.9999	1.05	3.00	1.23
<b>PL-20</b>	$y=3.5551x+402.64$	0.9999	0.20	1.00	16.76
<b>PL-21</b>	$y=3.0005x+358.81$	0.9994	0.25	1.00	2.96
<b>PL-22</b>	$y=3.7227x+507.26$	0.9992	0.10	0.50	8
<b>PL-23</b>	$y=5.0763x+911.53$	0.9999	0.15	0.50	3.86
<b>PL-24</b>	$y=14.782x-325.51$	0.9985	1.00	2.50	10.93
<b>PL-25</b>	$y=38.044x+1771.8$	0.9992	1.50	2.50	1.27
<b>PL-26</b>	$y=26.457x+1630.9$	0.9998	2.00	4.50	0.81
<b>PL-27</b>	$y=27.119x+388.22$	0.9999	0.50	2.50	2.37

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<b>PL-28</b>	$y=15.488x+143.07$	0.9994	0.05	0.30	1.59
<b>PL-29</b>	$y=8.1514x+1128.4$	0.9992	0.10	0.25	4.72

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<sup>a</sup>  $y$  is the peak area,  $x$  is the concentration ( $\mu\text{g/mL}$ )

**NMR data:****PL-1:** *diglucosylidirhamnoside*

<sup>13</sup>C NMR (151 MHz, Deuterium Oxide)  $\delta$  104.4 (C-1), 75.0 (C-2), 72.8(C-3), 71.0(C-4), 82.7(C-5), 62.2 (C-6), 101.5 (C-1'), 74.5 (C-2'), 72.8 (C-3'), 70.6 (C-4'), 76.9 (C-5'), 60.8 (C-6'), 98.1 (C-1''), 74.2 (C-2''), 72.5 (C-3''), 70.3 (C-4''), 76.1 (C-5''), 19.8 (C-6''), 92.1 (C-1'''), 74.2 (C-2'''), 72.2 (C-3'''), 69.7 (C-4'''), 75.1 (C-5'''), 17.6 (C-6'''). <sup>1</sup>H NMR (600 MHz, Deuterium Oxide)  $\delta$  5.20 (1H, d,  $J = 8.4$  Hz, H-1), 5.17 (1H, d,  $J = 3.3$  Hz, H-1'), 5.04 (1H, d,  $J = 9.0$  Hz, H-1''), 4.66 (1H, d,  $J = 6.6$  Hz, H-1'''), 4.45 (2H, m, H-5, 5'), 4.24 (2H, m, H-5'', 5'''), 3.96 (1H, m, H-2), 3.78 (1H, m, H-2'), 3.75 (1H, m, H-2''), 3.62 (1H, m, H-2'''), 3.54 (2H, m, H-3, 3'), 3.42 (2H, m, H-3'', 3'''), 3.18 (2H, m, H-4, 4'), 3.14 (2H, m, H-4'', 4'''), 3.11 (2H, m, H-6), 3.03 (2H, m, H-6'), 1.06 (3H, d,  $J = 5.7$  Hz, Me-6''), 0.87 (3H, d,  $J = 4.2$  Hz, Me-6''').

**PL-2:** *rutin*

<sup>13</sup>C NMR (151 MHz, Methanol-*d*4)  $\delta$  157.9 (C-2), 134.3 (C-3), 178 (C-4), 104.6 (C-4a), 161.6 (C-5), 98.7 (C-6), 164.3 (C-7), 93.5 (C-8), 158 (C-8a), 121.7 (C-1'), 114.7 (C-2'), 144.6 (C-3'), 148.5 (C-4'), 116.3 (C-5'), 122.2 (C-6'), 103.4 (C-1''), 74.4 (C-2''), 76.8 (C-3''), 70 (C-4''), 75.9 (C-5''), 67.2 (C-6''), 101 (C-1'''), 70.8 (C-2'''), 70.9 (C-3'''), 72.6 (C-4'''), 68.4 (C-5'''), 16.5 (C-6'''). <sup>1</sup>H NMR (600 MHz, Methanol-*d*4)  $\delta$  7.64 (d,  $J = 2.2$  Hz, 1H, H-2'), 7.61 (dd,  $J = 8.4, 2.2$  Hz, 1H, H-3'), 6.85 (d,  $J = 8.4$  Hz, 1H, H-6'), 6.37 (d,  $J = 2.1$  Hz, 1H, H-8), 6.18 (d,  $J = 2.1$  Hz, 1H, H-6), 5.08 (d,  $J = 7.7$  Hz, 1H, H-1''), 4.49 (d,  $J = 1.7$  Hz, 1H, H-1'''), 3.78-3.21 (m, glycoside), 1.10 (d,  $J = 6.2$  Hz, 3H, H-6''').

**PL-3:** *melibiose*

$^{13}\text{C}$  NMR (151 MHz, Deuterium Oxide)  $\delta$  98.68 (galactose C-1), 68.3 (C-2), 69.8 (C-3), 68.4 (C-4), 70.7 (C-5), 60.8 (C-6), 92.1 ( $\alpha$ -glucose C-1'), 72.1 (C-2'), 73.1 (C-3'), 70.1 (C-4'), 70.3 (C-5'), 67 (C-6'), 96 ( $\beta$ -glucose C-1'), 74.9 (C-2'), 75.8 (C-3'), 69.5 (C-4'), 74.8 (C-5'), 66.3 (C-6').  $^1\text{H}$  NMR (600 MHz, Deuterium Oxide)  $\delta$  4.83 (d,  $J$  = 1.7 Hz, 2H, H-1, 1'), 4.07 – 3.91 (m, 2H, H-5, 5'), 3.94 – 3.85 (m, 4H, H-6, 6'), 3.79 – 3.63 (m, 1H, H-3, 3'), 3.49 (dd,  $J$  = 9.2, 3.8 Hz, 2H, H-2, 2'), 3.48 – 3.44 (m, 2H, H-4, 4').

**PL-4:** *neryl-1-O- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 2)-O-[ $\alpha$ -L-arabinopyranosyl-(1 $\rightarrow$ 6)]-O- $\beta$ -D-glucopyranoside*

$^{13}\text{C}$  NMR (151 MHz, Deuterium Oxide)  $\delta$  66.2 (C-1), 119.3 (C-2), 141.2 (C-3), 39.2 (C-4), 35.8 (C-5), 122.8 (C-6), 131.3 (C-7), 24.8 (C-8), 14.3 (C-9), 16.7 (C-10), 100.7 (C-1'), 82.7 (C-2'), 75.7 (C-3'), 69.7 (C-4'), 76.1 (C-5'), 68.6 (C-6'), 103.6 (C-1''), 74.1 (C-2''), 76.1 (C-3''), 70.5 (C-4''), 76.7 (C-5''), 60.8 (C-6''), 103.2 (C-1'''), 71.5 (C-2'''), 72.8 (C-3'''), 68.6 (C-4'''), 65.3 (C-5''').  $^1\text{H}$  NMR (600 MHz, Deuterium Oxide)  $\delta$  5.4 (t, 1H,  $J$  = 6.4 Hz, H-1'), 5.19 (t, 2H,  $J$  = 7.1 Hz, H-1'', 1'''), 4.13 (t,  $J$  = 6.9 Hz, 2H, H-2,6), 3.98 (d,  $J$  = 15.4 Hz, 1H, H-2'', 2'''), 3.92 – 3.28 (m, 15H, H-2', 3', 4', 5', 6', 3'', 4'', 5'', 6'', 3''', 4''', 5'''), 1.69 – 1.62 (m, 2H, H-4, 5), 1.33 – 1.15 (m, 3H, H-8, 9, 10).

**PL-5:**  *$\beta$ -D-apiofuranosyl-(1 $\rightarrow$ 6)- $\beta$ -D-(1-O-methyl)-glucopyranoside*

$^{13}\text{C}$  NMR (151 MHz, Deuterium Oxide)  $\delta$  103.2 (C-1), 72.0 (C-2), 75.9 (C-3), 69.7 (C-4), 74.9 (C-5), 67.6 (C-6), 57.2 (C-7), 108.2 (C-1'), 76.8 (C-2'), 81.2 (C-3'), 73.1 (C-



4'), 62.5 (C-5'). <sup>1</sup>H NMR (600 MHz, Deuterium Oxide) δ 4.33 (d, *J* = 8.6 Hz, 1H, H-1'), 4.13 (s, 1H, H-1), 4.06 (s, 1H, H-2'), 4.01 (t, *J* = 8.0 Hz, 1H, H-2), 3.98 – 3.90 (m, 1H, H-4'), 3.83 (d, *J* = 12.2 Hz, 3H, H-4', 5'), 3.75 (d, *J* = 14.7 Hz, 5H, H-3, 4, 5, 6), 3.42 (dd, *J* = 17.7, 7.8 Hz, 3H, H-7).

**PL-6:** *N-vanillyl-nonanamide-β-lactoside*

<sup>13</sup>C NMR (151 MHz, Deuterium Oxide) δ 130.2 (C-1), 110.5 (C-2), 147.8 (C-3), 130.2 (C-4), 115.8 (C-5), 119.9 (C-6), 56.2 (C-7), 41.6 (C-8), 172.1 (C-1'), 35.4 (C-2'), 25.1 (C-3'), 28.7 (C-4'), 28.4 (C-5'), 27.4 (C-6'), 31.8 (C-7'), 22.4 (C-8'), 15.2 (C-9'), 103.3 (C-1''), 75.9 (C-2''), 69.6 (C-4''), 60.8 (C-6''), 104 (C-1'''), 75.9 (C-2'''), 73.1 (C-3'''), 69.1 (C-4'''), 73.5 (C-5'''), 62.6 (C-6'''). <sup>1</sup>H NMR (600 MHz, Deuterium Oxide) δ 6.98 (dd, *J* = 19.3, 11.4 Hz, 1H, H-2), 6.84 – 6.76 (m, 1H, H-5), 6.75 – 6.70 (m, 1H, H-6), 5.95 – 5.82 (m, 1H, H-1''), 5.45 (d, *J* = 5.7 Hz, 1H, H-1'''), 4.58 (dd, *J* = 17.4, 8.0 Hz, 1H, H-8), 4.36 (q, *J* = 11.5, 9.2 Hz, 2H, H-2'', 2'''), 3.84 (d, *J* = 11.5 Hz, 1H, H-3''), 3.77 (dt, *J* = 18.0, 9.6 Hz, 1H, H-3'''), 3.65 (tdd, *J* = 24.5, 15.0, 7.1 Hz, 8H, H-7, 5'', 6'', 6'''), 3.51 – 3.28 (m, 1H, H-4''', 5'''), 3.27 (d, *J* = 12.3 Hz, 1H, H-4''), 2.25 (d, *J* = 26.6 Hz, 2H, H-2'), 1.71 – 1.43 (m, 2H, H-3'), 1.32 – 1.24 (m, 4H, H-4', 5'), 1.26 – 1.17 (m, 4H, H-6', 7', 8'), 0.84 (tdd, *J* = 34.0, 18.7, 9.1 Hz, 3H, H-9').

**PL-7:** *palmatoside B*

<sup>13</sup>C NMR (151 MHz, Deuterium Oxide) δ 71.6 (C-1), 49 (C-2, 3), 84.4 (C-4), 42 (C-5), 24.8 (C-6), 13.2 (C-7), 39.7 (C-8), 35.7 (C-9), 53.6 (C-10), 47.2 (C-11), 68.9 (C-12), 123.6 (C-13), 108.5 (C-14), 143.7 (C-15), 140.2 (C-16), 175.5 (C-17), 169.3 (C-18), 30.4 (C-19), 21.6 (C-20), 99.5 (C-1'), 73.4 (C-2'), 76.6 (C-3'), 69.4 (C-4'), 76.2 (C-5'),

60.6 (C-6'). <sup>1</sup>H NMR (600 MHz, Deuterium Oxide) δ 7.63 (dd, *J* = 22.5, 7.9 Hz, 1H, H-15), 7.37 (d, *J* = 3.1 Hz, 1H, H-16), 6.84 (tdd, *J* = 15.8, 10.1, 7.1 Hz, 1H, H-14), 5.55 (d, *J* = 9.2 Hz, 1H, H-12), 5.39 (s, 1H, H-1'), 4.96 (d, *J* = 6.9 Hz, 1H, H-1), 4.07 – 4.01 (m, 1H, H-3), 3.80 – 3.54 (m, 7H, H-2,2',3',4',5',6'), 2.16 – 1.93 (m, 4H, H-8,7,11), 1.52 (s, 2H, H-6,7,10), 1.22 (s, 1H, H-20), 0.83 (s, 1H, H-19).

**PL-8:** *trans-3-hydroxy-1,8-cineole 3-O-β-D-glucopyranoside*

<sup>13</sup>C NMR (151 MHz, Deuterium Oxide) δ 72.7 (C-1), 41 (C-2), 71.5 (C-3), 35.1 (C-4), 12.9 (C-5), 29.8 (C-6), 25.2 (C-7), 74.8 (C-8), 27.2 (C-9), 28.5 (C-10), 100.6 (C-1'), 73.1 (C-2'), 75.9 (C-3'), 69.6 (C-4'), 75.7 (C-5'), 60.7 (C-6'). <sup>1</sup>H NMR (600 MHz, Deuterium Oxide) δ 5.22 (d, *J* = 3.8 Hz, 1H, H-1'), 3.79 – 3.61 (m, 5H, H-2', 3', 4', 5', 6'), 3.33 – 3.17 (m, 1H, H-3), 1.56 (d, *J* = 14.7 Hz, 4H, H-2, 6), 1.54 – 1.47 (m, 3H, H-4, 5), 1.26 – 1.10 (m, 6H, H-9, 10), 1.08 (s, 1H, H-7).

**PL-9:** *robinin*

<sup>13</sup>C NMR (151 MHz, Methanol-*d*4) δ 157.8 (C-2), 135.4 (C-3), 178.9 (C-4), 105.1 (4a), 162.4 (C-5), 99 (C-6), 165.1 (C-7), 93.9 (C-8), 158.5 (C-8a), 122 (C-1'), 131.2 (C-2'), 115.6 (C-3'), 160.7 (C-4'), 116.1 (C-5'), 131.2 (C-6'), 102.2 (C-1''), 69.7 (C-2''), 70.2 (C-3''), 71.7 (C-4''), 67.7 (C-5''), 16.9 (C-6''), 99 (C-1'''), 69.2 (C-2'''), 70.2 (C-3'''), 71.2 (C-4'''), 69.7 (C-5'''), 16.9 (C-6'''), 102.8 (C-1'''), 71.1 (C-2'''), 72.4 (C-3'''), 67.7 (C-4'''), 73.7 (C-5'''), 65.3 (C-6'''). <sup>1</sup>H NMR (600 MHz, Methanol-*d*4) δ 8.18(d, 2H, *J*=8.9 Hz, H-2', 6'), 6.81(d, 1H, H-8), 6.78(d, 2H, *J*=8.8 Hz, H-3', 5'), 6.43(d, 1H, H-6), 5.57(d, 1H, H-1'''), 5.36(d, 1H, H-1''), 4.30 (s, 1H, H-1'''), 1.28 – 1.15 (m, 12H, other glycoside proton signal), 1.15 – 1.10 (m, 6H, H-6''', 6''').

**PL-10:** *phenyl-β-D-glucoopyranoside*

<sup>13</sup>C NMR (151 MHz, Deuterium Oxide) δ 154.9 (C-1), 115.2 (C-2, 6), 128.8 (C-3, 5), 132.2 (C-4), 102.3 (C-1'), 73.1 (C-2'), 75.8 (C-3'), 69.7 (C-4'), 75.9 (C-5'), 60.8 (C-6'). <sup>1</sup>H NMR (600 MHz, Deuterium Oxide) δ 7.11 (d, *J* = 7.7 Hz, 2H, H-3, 5), 7.0 (d, *J* = 10 Hz, 3H, H-2, 4, 6), 4.87 (d, *J* = 7.4 Hz, 1H, H-1'), 3.91-3.73 (dd, *J* = 12.1 Hz, 2H, H-6'), 3.40 - 3.50 (m, 4H, H-2', 3', 4', 5').

**PL-11:** *euodionoside D*

<sup>13</sup>C NMR (151 MHz, Methanol-*d*<sub>4</sub>) δ 40.5 (C-1), 45 (C-2), 65.3 (C-3), 44.2 (C-4), 76.4 (C-5), 77.5 (C-6), 133.3 (C-7), 131.6 (C-8), 76.3 (C-9), 22.4 (C-10), 27.6 (C-11), 26.2 (C-12), 28.5 (C-13), 101.2 (C-1'), 74 (C-2'), 77 (C-3'), 70.4 (C-4'), 76.6 (C-5'), 63.9 (C-6'). <sup>1</sup>H NMR (600 MHz, Methanol-*d*<sub>4</sub>) δ 6.08-5.89 (m, 2H, H-7,8), 5.42 (s, 1H, H-1'), 4.03 – 3.91 (m, 1H, H-9), 3.91 – 3.73 (m, 6H, H-2',3',4',5',6'), 3.43 – 3.33 (m, 1H, H-3), 2.03 – 1.89 (m, 2H, H-4), 1.79 – 1.52 (m, 2H, H-2), 1.24 – 1.18 (m, 3H, H-13), 1.20 – 1.08 (m, 4H, H-10), 0.82 (s, 6H, H-11,12).

**PL-12:** *germacradiene-6-O-(6'-O-acetyl)-β-D-glucoside*

<sup>13</sup>C NMR (151 MHz, Methanol-*d*<sub>4</sub>) δ 132.2 (C-1), 65.4 (C-2), 44.2 (C-3), 131.1 (C-4), 133.3 (C-5), 80.1 (C-6), 45 (C-7), 24.9 (C-8), 39.3 (C-9), 135.6 (C-10), 73.5 (C-11), 26.1 (C-12), 30 (C-13), 20.5 (C-14), 12.8 (C-15), 101.3 (C-1'), 73.7 (C-2'), 76.6 (C-3'), 70.4 (C-4'), 74 (C-5'), 63.9 (C-6'), 168.1 (C-7'), 18.9 (C-8'). <sup>1</sup>H NMR (600 MHz, Methanol-*d*<sub>4</sub>) δ 7.65 (dd, *J* = 5.7, 3.3 Hz, 1H, H-8), 7.55 (dd, *J* = 5.7, 3.3 Hz, 1H, H-9), 6.05 – 5.94 (m, 2H, H-1, 1'), 5.84 – 5.77 (m, 1H, H-5), 4.38 – 4.11 (m, 4H, H-2, 2', 5', 6'), 3.92 – 3.82 (m, 1H, H-3'), 3.80 (s, 1H, H-4'), 2.36 – 2.24 (m, 2H, H-3, 14), 2.06 –

1.94 (m, 1H, H-8'), 1.88 (dddd,  $J = 14.8, 11.6, 5.2, 3.4$  Hz, 3H, H-15), 1.09 (d,  $J = 1.3$  Hz, 6H, H-12, 13).

**PL-13:** *ethyl  $\alpha$ -L-rhamnopyranosyl-(1 $\rightarrow$ 6)- $\beta$ -D-glucoside*

$^{13}\text{C}$  NMR (151 MHz, Methanol- $d_4$ )  $\delta$  101 (C-1), 70.8 (C-2), 71 (C-3), 72.7 (C-4), 68.4 (C-5), 16.7 (C-6), 102.8 (C-1'), 73.7 (C-2'), 76.7 (C-3'), 70.3 (C-4'), 75.5 (C-5'), 66.9 (C-6'), 64.9 (C-7'), 14.2 (C-8').  $^1\text{H}$  NMR (600 MHz, Methanol- $d_4$ )  $\delta$  4.72 (d, 1H, H-1'), 4.07 (d, 1H, H-1), 3.95 (d, 1H, H-2'), 3.93 (d, 1H, H-2), 3.80 (dd, 2H, H-3', 5'), 3.71 (d, 2H, H-7'), 3.6-3.56 (m, 2H, H-6'), 3.50 (m, 2H, H-3, 5), 3.29 (m, 1H, H-4'), 3.13 (d, 1H, H-4), 1.25 – 1.10 (m, 6H, H-6, 8').

**PL-14:** *olaximbricide D*

$^{13}\text{C}$  NMR (151 MHz, Methanol- $d_4$ )  $\delta$  27.6 (C-1), 41.5 (C-2), 24.9 (C-3), 26.7 (C-4), 153.7 (C-5), 114.9 (C-6), 127 (C-7), 130 (C-8), 136.6 (C-9), 126.2 (C-10), 74 (C-11), 69.9 (C-12), 22.5 (C-13), 20.2 (C-14), 101.3 (C-1'), 73.4 (C-2'), 77.8 (C-3'), 70 (C-4'), 76.6 (C-5'), 61.1 (C-6').  $^1\text{H}$  NMR (600 MHz, Methanol- $d_4$ )  $\delta$  6.79 (dd,  $J = 8.6, 2.2$  Hz, 2H, H-6, 7), 5.84 (dd,  $J = 16.6, 6.7$  Hz, 1H, H-1'), 4.18 – 4.11 (m, 1H, H-2'), 3.95 (dddd,  $J = 15.3, 11.6, 8.1, 4.8$  Hz, 1H, H-3'), 3.82 (s, 1H, H-4', 5'), 3.57 (m, 1H, H-6'), 3.21 – 3.05 (m, 7H, H-1, 4), 2.05 – 1.94 (m, 1H, H-14), 1.67 (s, 1H, H-3), 1.42 – 1.36 (m, 1H, H-2), 1.19 (d,  $J = 8.2$  Hz, 3H, H-13).

**PL-15:** *puerarin*

$^{13}\text{C}$  NMR (100 MHz, Methanol- $d_4$ )  $\delta$  154.3 (C-2), 125.3 (C-3), 178.1 (C-4), 118.2 (C-4a), 127.9 (C-5), 116 (C-6), 162.9 (C-7), 113 (C-8), 158.5 (C-8a), 124 (C-1'), 131.2 (C-2', 6'), 116 (C-3', 5'), 158.5 (C-4'), 75.4 (C-1''), 72.7 (C-2''), 79.8 (C-3''), 71.5 (C-

4''), 82.5 (C-5''), 62.6 (C-6''). <sup>1</sup>H NMR (400 MHz, Methanol-*d*<sub>4</sub>) δ 8.17 (s, 1H, H-2), 8.03 (d, *J* = 8.8 Hz, 1H, H-5), 7.39 – 7.31 (m, 2H, H-2', 6'), 6.97 (d, *J* = 8.8 Hz, 1H, H-6), 6.87 – 6.79 (m, 2H, H-3', 5'), 5.08 (d, *J* = 9.9 Hz, 1H, H-1''), 4.11 (s, 1H, H-2''), 3.74 (dd, *J* = 12.1, 5.1 Hz, 1H, H-3''), 3.50 (td, *J* = 7.9, 7.4, 2.5 Hz, 2H, H-4'', 5''), 3.46 (s, 1H, H-6'').

**PL-16:** *daidzin*

<sup>13</sup>C NMR (151 MHz, Methanol-*d*<sub>4</sub>) δ 153.7 (C-2), 124.9 (C-3), 176.7 (C-4), 118.9 (C-4a), 127 (C-5), 115.7 (C-6), 162.2 (C-7), 103.6 (C-8), 157.5 (C-8a), 122.7 (C-1'), 130 (C-2', 6'), 114.9 (C-3', 5'), 157.7 (C-4'), 100.5 (C-1''), 73.4 (C-2''), 77 (C-3''), 69.9 (C-4''), 76.5 (C-5''), 61.1 (C-6''). <sup>1</sup>H NMR (600 MHz, Methanol-*d*<sub>4</sub>) δ 8.18 (s, 1H, H-2), 8.12 (d, *J* = 8.9 Hz, 1H, H-5), 7.38 – 7.34 (m, 2H, H-2', 6'), 7.23 (d, *J* = 2.3 Hz, 1H, H-8), 7.19 (dd, *J* = 8.9, 2.3 Hz, 1H, H-6), 6.85 – 6.80 (m, 2H, H-3', 5'), 5.10 – 5.06 (m, 1H, H-1''), 3.42 – 3.90 (m, 6H, H-2'' ~ 6'').

**PL-17:** *daidzein*

<sup>13</sup>C NMR (151 MHz, DMSO-*d*<sub>6</sub>) δ 153.8 (C-2), 124 (C-3), 173.7 (C-4), 117.1 (C-4a), 126.8 (C-5), 115.6 (C-6), 162.6 (C-7), 102.6 (C-8), 157.9 (C-8a), 122.9 (C-1'), 130.6 (C-2', 6'), 115.4 (C-3', 5'), 157.7 (C-4'). <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 10.75 (s, 1H, 7-OH), 9.49 (s, 1H, 4'-OH), 8.25 (s, 1H, H-2), 7.92 (d, *J* = 8.8 Hz, 1H, H-5), 7.36 – 7.32 (m, 2H, H-2', 6'), 6.89 (dd, *J* = 8.8, 2.3 Hz, 1H, H-8), 6.82 (d, *J* = 2.3 Hz, 1H, H-6), 6.78 – 6.74 (m, 2H, H-3', 5').

**PL-18:** *viburtinoside IV*

<sup>13</sup>C NMR (151MHz, Methanol-*d*<sub>4</sub>) δ 92.6 (C-1), 133.4 (C-2), 116.5 (C-3), 32.1 (C-4),

39.3 (C-5), 81.9 (C-6), 82.8 (C-7), 44.9 (C-8), 64.6 (C-9), 170.6 (C-10), 68.2 (C-11), 173.2 (C-12), 44.2 (C-13), 26.2 (C-14), 24.9 (C-15, 16), 69.9 (C-17), 101.2 (C-1'), 75.4 (C-2'), 76.6 (C-3'), 70.5 (C-4'), 77.5 (C-5'), 63.1 (C-6'), 170.6 (C-7'), 20.5 (C-8'). <sup>1</sup>H NMR (600 MHz, Methanol-*d*<sub>4</sub>) δ 6.06 (dd, *J* = 15.9, 1.0 Hz, 1H, H-1), 5.85 – 5.78 (m, 2H, H-1', 2), 4.42 – 4.30 (m, 2H, H-2'), 4.07 – 3.97 (m, 4H, H-9, 17), 3.97 – 3.91 (m, 1H, H-3'), 3.90 – 3.44 (m, 4H, H-6, 4', 5', 6'), 1.82 – 1.66 (m, 2H, H-8, 14), 1.41 (ddd, *J* = 12.3, 4.3, 2.0 Hz, 1H, H-13), 1.30 (s, 4H, H-4, 11, 8'), 1.31 – 1.21 (m, 2H, H-5), 1.08 (d, *J* = 2.4 Hz, 6H, H-15, 16).

**PL-19:** *(3R,9R)-5-megastigmen-3, 9, 11-triol 9-O-β-D-glucopyranoside*

<sup>13</sup>C NMR (151 MHz, Deuterium Oxide) δ 48.5 (C-1), 43.9 (C-2), 64.1 (C-3), 43.1 (C-4), 131.4 (C-5), 134.1 (C-6), 25.1 (C-7), 39.1 (C-8), 76 (C-9), 20.4 (C-10), 69.7 (C-11), 24.7 (C-12), 20.9 (C-13), 100.6 (C-1'), 75.7 (C-2'), 78.2 (C-3'), 72.7 (C-4'), 76.8 (C-5'), 60.6 (C-6'). <sup>1</sup>H NMR (600 MHz, Deuterium Oxide) δ 4.54 (d, *J* = 8.0 Hz, 1H, H-1'), 3.86 – 3.81 (m, 1H, H-3), 3.72 (s, 1H, H-3'), 3.74 – 3.66 (m, 2H, H-4', 5'), 3.34 (s, 2H, H-11, 6'), 3.32 – 3.24 (m, 1H, H-9), 3.27 – 3.20 (m, 1H, H-4), 1.91 – 1.85 (m, 2H, H-7), 1.69 (ddd, *J* = 13.1, 11.8, 1.2 Hz, 2H, H-2), 1.60 – 1.52 (m, 3H, H-13), 1.34 (dd, *J* = 6.4, 0.9 Hz, 5H, H-8, 10), 0.84 (s, 3H, H-12).

**PL-20:** *8-debenzoylpaeoniflorin*

<sup>13</sup>C NMR (151 MHz, Deuterium Oxide) δ 88.1 (C-1), 94.2 (C-2), 43.5 (C-3), 106.1 (C-4), 42.7 (C-5), 75.2 (C-6), 24.3 (C-7), 60.1 (C-8), 103.2 (C-9), 19.9 (C-10), 100.1 (C-1'), 72.9 (C-2'), 78.1 (C-3'), 75.5 (C-4'), 77.8 (C-5'), 63.6 (C-6'). <sup>1</sup>H NMR (600 MHz, Deuterium Oxide) δ 5.84 (dd, *J* = 15.9, 7.4 Hz, 2H, H-9, 1'), 4.55 (s, 1H, H-5), 4.10

(ddd,  $J = 8.5, 4.7, 2.6$  Hz, 2H, H-8), 3.88 - 3.82 (m, 2H, H-6'), 3.41-3.37 (m, 3H, H-8,3'), 3.35 (s, 1H, H-2'), 3.29-3.22 (m, 2H, H-4',5'), 1.93-1.86 (m, 2H, H-7), 1.74-1.67 (m, 2H, H-3), 1.35 (s, 3H, H-10).

**PL-21:** *raffinose*

$^{13}\text{C}$  NMR (151 MHz, Deuterium Oxide)  $\delta$  98.1 (C-1), 71.4 (C-2), 72.7 (C-3), 69.2 (C-4), 75.9 (C-5), 60 (C-6), 90.6 (C-1'), 71.6 (C-2'), 65.3 (C-3'), 70.5 (C-4'), 82.7 (C-5'), 63.4 (C-6'), 103.8 (C-1''), 69.6 (C-2''), 69.8 (C-3''), 73.1 (C-4''), 67.5 (C-5''), 60.7 (C-6'').  $^1\text{H}$  NMR (600 MHz, Deuterium Oxide)  $\delta$  5.53(m, 2H, H-1,1'), 4.19 – 3.17 (m, remaining proton signal).

**PL-22:** *6-hydroxyhexyl  $\beta$ -D-glucopyranoside*

$^{13}\text{C}$  NMR (151 MHz, Deuterium Oxide)  $\delta$  69.7 (C-1), 27.7 (C-2), 27.5 (C-3), 26.5 (C-4), 32.4 (C-5), 60.8 (C-6), 102.9 (C-1'), 73.8 (C-2'), 75.8 (C-3'), 73.1 (C-4'), 75.9 (C-5'), 60.6 (C-6').  $^1\text{H}$  NMR (600 MHz, Deuterium Oxide)  $\delta$  3.87 – 3.71 (m, 1H, H-1'), 3.73 (s, 2H, H-2'), 3.70 – 3.54 (m, 3H, H-4', 5', 6), 3.56 – 3.50 (m, 2H, H-3'), 3.50 – 3.20 (m, 2H, H-1), 1.18 – 1.07 (m, 1H, H-6), 1.12 (s, 1H, H-6'), 1.07 – 0.95 (m, 4H, H-2, 3, 4, 5).

**PL-23:**  *$\beta$ -D-fructopyranosyl-(2 $\rightarrow$ 6)- $\alpha$ -D-glucopyranosyl-(1 $\leftrightarrow$ 2)- $\beta$ -D-fructofuranoside*

$^{13}\text{C}$  NMR (151 MHz, Deuterium Oxide)  $\delta$  62.5 (C-1), 103.2 (C-2), 76 (C-3), 74.5 (C-4), 82.7 (C-5), 63.3 (C-6), 62.4 (C-1'), 101.5 (C-2'), 69.2 (C-3'), 70.5 (C-4'), 69.8 (C-5'), 64 (C-6'), 92.1 (C-1''), 71.7 (C-2''), 73.1 (C-3''), 69.7 (C-4''), 72.1 (C-5''), 59.7 (C-6'').  $^1\text{H}$  NMR (600 MHz, Deuterium Oxide)  $\delta$  5.22 (d,  $J = 3.9$  Hz, 1H, H-1''). 4.10 (dd,  $J = 3.8, 0.9$  Hz, 1H, H-3), 4.01 (dd,  $J = 12.7, 1.5$  Hz, 1H, H-4), 3.99 (t,  $J = 2.8$  Hz,

2H, H-5', 6'), 3.99 – 3.97 (m, 1H, H-3', 4'), 3.90 (dd,  $J = 10.9, 4.2$  Hz, 1H, H-5''), 3.88 (dd,  $J = 10.1, 3.5$  Hz, 1H, H-5), 3.83 – 3.77 (m, 2H, H-6, 1'), 3.77 – 3.69 (m, 3H, H-3'', 6''), 3.70 – 3.64 (m, 2H, H-1), 3.34 (s, 2H, H-2'', 4'').

**PL-24:** *quercetin*

$^{13}\text{C}$  NMR (151 MHz, Methanol- $d_4$ )  $\delta$  156.8 (C-2), 135.9 (C-3), 175.9 (C-4), 103.2 (C-4a), 161.1 (C-5), 97.9 (C-6), 164.2 (C-7), 93.1 (C-8), 147.4 (C-8a), 120.3 (C-1'), 114.8 (C-2'), 144.9 (C-3'), 146.6 (C-4'), 114.6 (C-5'), 122.4 (C-6').  $^1\text{H}$  NMR (600 MHz, Methanol- $d_4$ )  $\delta$  7.71 (d,  $J = 2.2$  Hz, 1H, H-2'), 7.61 (dd,  $J = 8.5, 2.2$  Hz, 1H, H-6'), 6.86 (d,  $J = 8.5$  Hz, 1H, H-5'), 6.36 (d,  $J = 2.1$  Hz, 1H, H-6), 6.15 (d,  $J = 2.1$  Hz, 1H, H-8).

**PL-25:** *quercitrin*

$^{13}\text{C}$  NMR (151 MHz, Methanol- $d_4$ )  $\delta$  157.2 (C-2), 134.9 (C-3), 178.3 (C-4), 104.5 (C-4a), 158 (C-5), 98.5 (C-6), 164.6 (C-7), 93.4 (C-8), 161.9 (C-8a), 121.6 (C-1'), 115 (C-2'), 145.1 (C-3'), 148.5 (C-4'), 115.6 (C-5'), 121.5 (C-6'), 102.2 (C-1''), 70.7 (C-2''), 3''), 71.9 (C-4''), 70.5 (C-5''), 16.3 (C-6'').  $^1\text{H}$  NMR (600 MHz, Methanol- $d_4$ )  $\delta$  7.31 (d,  $J = 2.1$  Hz, 1H, H-2'), 7.28 (dd,  $J = 8.3, 2.1$  Hz, 1H, H-6'), 6.88 (d,  $J = 8.3$  Hz, 1H, H-5'), 6.35 (d,  $J = 2.1$  Hz, 1H, H-6), 6.18 (d,  $J = 2.1$  Hz, 1H, H-8), 5.32 (s, 1H, H-1''), 4.19 (dd,  $J = 3.4, 1.7$  Hz, 1H, H-2''), 3.71 (d,  $J = 3.3$  Hz, 2H, H-3'', 4''), 3.31 (d,  $J = 10.0$  Hz, 1H, H-5''), 0.91 (d,  $J = 6.2$  Hz, 3H, H-6'').

**PL-26:** *isoquercitrin*

$^{13}\text{C}$  NMR (151 MHz, Methanol- $d_4$ )  $\delta$  157.2 (C-2), 134.2 (C-3), 178.1 (C-4), 104.3 (C-4a), 161.8 (C-5), 98.5 (C-6), 164.7 (C-7), 93.3 (C-8), 157.7 (C-8a), 121.8 (C-1'), 114.6



(C-2'), 144.3 (C-3'), 148.7 (C-4'), 116.2 (C-5'), 122.4 (C-6'), 102.8 (C-1''), 74.4 (C-2''), 76.8 (C-3''), 69.8 (C-4''), 77.1 (C-5''), 61.2 (C-6''). <sup>1</sup>H NMR (600 MHz, Methanol-*d*<sub>4</sub>) δ 7.68 (d, *J* = 2.2 Hz, 1H, H-2'), 7.57 (dd, *J* = 8.5, 2.2 Hz, 1H, H-6'), 6.84 (d, *J* = 8.5 Hz, 1H, H-5'), 6.38 (d, *J* = 2.2 Hz, 1H, H-8), 6.18 (d, *J* = 2.2 Hz, 1H, H-6), 5.25 (s, 1H, H-1''), 3.69 (dd, *J* = 11.9, 2.4 Hz, 1H, H-6''), 3.55 (dd, *J* = 11.9, 5.4 Hz, 1H, H-2''), 3.45 (dd, *J* = 9.2, 7.7 Hz, 1H, H-3''), 3.43 – 3.37 (m, 1H, H-4''), 3.35 – 3.28 (m, 1H, H-5'').

**PL-27:** *esculin*

<sup>13</sup>C NMR (151 MHz, Methanol-*d*<sub>4</sub>) δ 162.3 (C-2), 111.8 (C-3), 144.7 (C-4), 111.5 (C-4a), 115.2 (C-5), 143.1 (C-6), 151.2 (C-7), 103.2 (C-8), 151.9 (C-8a), 103 (C-1'), 73.4 (C-2'), 77.2 (C-3'), 70 (C-4'), 76.2 (C-5'), 61.1 (C-6'). <sup>1</sup>H NMR (600 MHz, Methanol-*d*<sub>4</sub>) δ 7.82 (dd, *J* = 9.6, 0.6 Hz, 1H, H-4), 7.42 (s, 1H, H-5), 6.79 (d, *J* = 0.6 Hz, 1H, H-8), 6.20 (d, *J* = 9.4 Hz, 1H, H-3).

**PL-28:** *kaempferol*

<sup>13</sup>C NMR (151 MHz, Methanol-*d*<sub>4</sub>) δ 148.9 (C-2), 136.8 (C-3), 170.2 (C-4), 106.7 (C-4a), 153.6 (C-5), 96.6 (C-6), 164.5 (C-7), 93.9 (C-8), 151 (C-8a), 121.8 (C-1'), 126.6 (C-2'), 113.2 (C-3'), 156.3 (C-4'), 113.2 (C-5'), 126.6 (C-6'). <sup>1</sup>H NMR (600 MHz, Methanol-*d*<sub>4</sub>) δ 8.09 – 8.05 (m, 2H, H-2', 6'), 6.90 – 6.86 (m, 2H, H-3', 5'), 6.38 (d, *J* = 2.1 Hz, 1H, H-8), 6.16 (d, *J* = 2.1 Hz, 1H, H-6).

**PL-29:** *arbutin*

<sup>13</sup>C NMR (151 MHz, Deuterium Oxide) δ 155.7 (C-1), 115.5 (C-2, 6), 120.1 (C-3, 5), 153.4 (C-4), 101.5 (C-1'), 74.3 (C-2'), 78.2 (C-3'), 69.7 (C-4'), 78.2 (C-5'), 61.1 (C-6').

$^1\text{H}$  NMR (600 MHz, Deuterium Oxide)  $\delta$  7.75 (d,  $J = 9.1$  Hz, 2H, H-3, 5), 7.20 (d,  $J = 8.4$  Hz, 2H, H-2, 6), 6.67 (d,  $J = 9.1$  Hz, 1H, H-1'), 4.94 (d,  $J = 10.0$  Hz, 1H, H-6').  
3.20-3.82 (other glycoside proton signal).