Supplementary Material

ISOLATION AND EVALUATION OF HEDGEHOG INHIBITORS FROM CHRISTMAS GRASS (*Themeda arguens*)

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Characteristic data of compounds (**1**–**4**).

aciculatin (**1**) yellow amorphous solid; $[\alpha]_D^{25}$ +13 (*c* 0.5, MeOH), ESIMS *m/z* 415 $[M+H]^+$, 437 $M+Na]^+$. ^{1}H-NMR (600 MHz, in $CDCl_3$:CD_3OD 1:1), δ: 7.97 (2H, d, *J* = 8.8 Hz, 2', 6'-H), 6.96 (2H, d, *J* = 8.8 Hz, 3', 5'-H), 6.59 (1H, s, 3-H), 6.44 (1H, s, 6-H), 5.64 (1H, d, *J* = 11.5 Hz, 1"-H), 4.16 (1H, d, *J* = 2.2 Hz, 3"-H), 3.96 (dd, *J* = 9.2, 6.2 Hz, 5"-H), 3.93 (3H, s, -OMe), 3.49 (1H, dd, *J* = 9.2, 2.2 Hz, 4"-H), 2.60 (1H, dd, *J* = 14.0, 11.5 Hz, 2"-H), 1.86 (1H, d, *J* = 14.0 Hz, 2"-H), 1.39 (3H, d, *J* = 6.2 Hz, 6"-H). ^{13}C-NMR (150 MHz, in $CDCl_3$:CD_3OD 1:1), δ: 164.9 (2-C), 162.5 (7-C), 160.9 (5-C), 155.3 (9-C), 128.4 (2', 6'-C), 128.3 (4'-C), 121.8 (1'-C), 115.4 (3', 5'-C), 106.9 (8-C), 102.2 (10-C), 102.1 (3-C), 93.6 (6-C), 73.1 (4"-C), 72.4 (5"-C), 67.3 (3"-C), 65.3 (1"-C), 55.5 (OMe), 35.8 (2"-C), 17.7 (5"-C).

8-*C*-β-D-digitoxopyranosylapigenin (**2**) yellow amorphous solid; $[\alpha]_D^{24}$ +101 (*c* 1.0, MeOH),ESIMS *m/z* 401 $[M+H]^+$. ^{1}H-NMR (600 MHz, in Acetone-d_6), δ: 12.95 (1H, s, 5-OH), 8.07 (2H, d, *J* = 8.8 Hz, 2', 6'-H), 7.01 (2H, d, *J* = 8.8 Hz, 3', 5'-H), 6.67 (1H, s, 3-H), 6.17 (1H, s, 6-H), 5.76 (1H, dd, *J* = 11.4 Hz, 1.8, 1"-H), 4.17 (1H, d, *J* = 2.0 Hz, 3"-H), 4.00 (1H, dq, *J* = 9.2, 6.4 Hz, 5"-H), 3.48 (dd, *J* = 9.2, 2.0 Hz, 4"-H), 2.20 (1H, dd, *J* = 14.0, 1.8 Hz, 2"-H), 2.14 (1H, dd, *J* = 14.0, 1.8 Hz, 2"-H), 1.38 (3H, d, *J* = 6.4 Hz, 6"-H). ^{13}C-NMR (150 MHz, in Acetone-d_6), δ: 183.2 (4-C), 164.7 (2-C), 163.2 (7-C), 162.1 (5-C), 162.1 (4'-C), 154.3 (9-C), 129.5 (2', 6'-C), 123.0 (1'-C), 116.9 (3', 5'-C), 105.4 (8-C), 105.2 (10-C), 103.6 (3-C), 100.3 (6-C), 74.7 (5"-C), 73.6 (4"-C), 68.0 (3"-C), 70.3 (1"-C), 38.9 (2"-C), 18.7 (6"-C).

8-*C*-β-D-boivinopyranosylapigenin (**3**) yellow amorphous solid; $[\alpha]_D^{24}$ +70 (*c* 0.2, MeOH), ESIMS *m/z* 401 $[M+H]^+$. ^{1}H-NMR (600 MHz, in Acetone-d_6), δ: 12.95 (1H, s, 5-OH), 8.01 (2H, d, *J* = 8.8 Hz, 2', 6'-H), 6.99 (2H, d, *J* = 8.8 Hz, 3', 5'-H), 6.65 (1H, s, 3-H), 6.17 (1H, s, 6-H), 5.76 (1H, dd, *J* = 12.0, 2.4 Hz, 1"-H), 4.28 (1H, q, *J* = 6.4 Hz, 5"-H), 4.11 (1H, d, *J* = 2.4 Hz, 3"-H), 3.52 (d, *J* = 2.4 Hz, 4"-H), 2.34 (1H, dd, *J* = 13.2, 12.0 Hz, 2"-H), 1.85 (1H, d, *J* = 13.2 Hz, 2"-H), 1.30 (3H, d, *J* = 6.4 Hz, 6"-H). ^{13}C-NMR (150 MHz, in Acetone-d_6), δ: 183.2 (4-C), 164.7 (2-C), 163.9 (7-C), 162.0 (5-C), 162.1 (4'-C), 154.0 (9-C), 129.4 (2', 6'-C), 123.0 (1'-C), 116.9 (3', 5'-C), 105.0 (8-C), 105.0 (10-C), 103.6 (3-C), 100.5 (6-C), 72.8 (5"-C), 70.3 (1"-C), 70.3 (4"-C), 68.2 (3"-C), 33.8 (2"-C), 17.3 (6"-C).

aciculatinone (**4**) yellow amorphous solid; $[\alpha]_D^{24}$ +79 (*c* 0.27, MeOH), ^{1}H data, Table, ESIMS *m/z* 413 $[M+H]^+$. ^{1}H-NMR (600 MHz, in Acetone-d_6), δ: 13.44 (1H, s, 5-OH), 8.08 (2H, d, *J* = 8.8 Hz, 2', 6'-H), 7.06 (2H, d, *J* = 8.8 Hz, 3', 5'-H), 6.70 (1H, s, 3-H), 6.49 (1H, s, 6-H), 5.40 (1H, dd, *J* = 12, 2.8 Hz, 1"-H), 4.09 (d, *J* = 10 Hz, 4"-H), 3.60 (1H, m, 5"-H), 3.55 (1H, dd, *J* = 12.0, 1.6 Hz, 2"-H), 2.51 (1H, dd, *J* = 13.6, 2.8 Hz, 2"-H), 1.48 (3H, d, *J* = 6.4 Hz, 6"-H).