Supporting Information

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Phytochemical Studies and Antioxidant Activities of

Artocarpus scortechinii King

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Experimental Details

Antioxidant Activities

2,2-Diphenyl-1-picrylhydrazyl (DPPH) assay: The DPPH assay was conducted according to method by Fu *et al.* with minor modification [1]. 100 μ L of DPPH stock solution (0.1 mM) was mixed with sample 100 μ L and incubated for 30 minutes in the dark at room temperature. The absorbance was measured using EPOCH microplate reader at 517 nm. The sample was replaced with methanol for blank sample. Percentage inhibition was calculated using the following formula:

Percentage inhibition = [(Absorbance blank DPPH–Absorbance sample)/ Absorbance blank DPPH] × 100%

2,2'-Azino-bis(3-ethylbenzthiazoline-6-sulphonic acid) (ABTS) assay: The ABTS assay was carried out based on method described by Zou *et al.* with minor modification [2]. ABTS and potassium persulfate were dissolved in distilled water to obtain concentration 7 mM and 4.9 mM respectively. Equal amount of these two solutions were mixed and let stand for 12 to 16 hours at room temperature before use. The ABTS radical was added with distilled water to absorbance of 0.7 at 734 nm. 10 μ L of sample was added to 96-well plates together with 190 μ L of ABTS solutions. The absorbance was recorded after 30 minutes incubation in the dark at room temperature. The percentage of antioxidant activity was calculated using the following formula:

Scavenging concentration = [Abs (ABTS)-Abs (ABTS+Sample)/Abs (ABTS)] × 100%

Ferric reducing antioxidant potential (FRAP) assay: Experiment was carried out according to Channarong *et al.* with minor modification [3]. FRAP reagent was freshly prepared, consist of stock solution with ratio 10:1:1 of 300 mM acetate buffer, 10 mM TPTZ in 40 mM HCl and 20 mM FeCl₃.6H₂O solution. 5 μ L of sample, 15 μ L of methanol and 150 μ L of FRAP reagent were added to the 96-well plates. The absorbance at 573 nm was read after 10 minutes of incubation at 37°C. FeSO₄.7H₂O solution (0.1 mM – 1.0 mM) was used to build up calibration curves of standard antioxidants.

Statistical Analysis of Data:

Three replicates of each sample were used for statistical analysis with values reported as mean \pm SD. Standard curves were generated and calculation of the 50% inhibitory concentration (IC₅₀) values was performed using GraphPad Prism for Windows (Version 5.02) software. The test was carried out using SPSS (version 16) software to study the comparison between treatment of samples and untreated control. A value of p < 0.05 was considered significantly different.

4',5-Dihydroxy-6,7-(2,2-dimethylpyrano)-2'-methoxy-8-γ,γ-dimethylallylflavone (**1**) : Pale yellow solid (66.7 mg, 1.67%). R_f 0.38 (*n*-Hex:EtOAc = 1:1); IR (ATR) v_{max} cm⁻¹: 3393 (OH), 2943 (sp^3 CH), 1649 (C=O), 1622 and 1561 (C=C aromatic), and 1208 (C-O); ¹H NMR (CD₃COCD₃, 400 MHz) ppm: δ 13.68 (1H, s, 5-OH), 7.73 (1H, d, J = 8.4 Hz, H-6'), 6.76 (1H, s, H-3), 6.73 (1H, dd, , J = 16.4 Hz and 7.2 Hz, H-10), 6.65 (1H, dd, J = 8.4 Hz and 2.4 Hz, H-5'), 6.60 (1H, d, J = 16.4 Hz, H-9), 6.45 (1H, d, J = 2.4 Hz, H-3'), 6.24 (1H, d, J = 9.2 Hz, H-14), 5.48 (1H, d, J = 9.2 Hz, H-15), 4.00 (3H, s, OCH₃), 2.45 (1H, m, H-11), 1.96 (3H, s, H-17), 1.70 (3H, s, H-18), 1.09 (6H, s, H-12 and H-13); ¹³C NMR (CD₃COCD₃, 100 MHz) ppm: δ 178.5 (C-4), 163.2 (C-4'), 162.7 (C-2'), 158.9 (C-8a), 155.7 (C-2), 155.3 (C-5), 141.7 (C-10), 138.0 (C-16), 125.4 (C-6'), 121.2 (C-15), 115.8 (C-9), 109.9 (C-5'), 109.5 (C-6), 109.2 (C-8), 107.5 (C-1'), 105.1 (C-4a), 104.0 (C-3'), 90.2 (C-3), 69.5 (C-14), 55.8 (O-CH₃), 33.1 (C-11), 24.9 (C-18), 22.2 (C-12 and C-13), 17.8 (C-17); EIMS m/z (% rel. int.): 434 [M]⁺, C₂₆H₂₆O₆.



S1: IR spectrum of 4',5-dihydroxy-6,7-(2,2-dimethylpyrano)-2'-methoxy-8- γ , γ -dimethylallylflavone (1)



S2: ¹H NMR spectrum of 4',5-dihydroxy-6,7-(2,2-dimethylpyrano)-2'-methoxy-8-γ,γdimethylallylflavone (**1**)



S3: ¹H NMR spectrum of 4',5-dihydroxy-6,7-(2,2-dimethylpyrano)-2'-methoxy-8-γ,γdimethylallylflavone (1) (Expansion)



S4: ¹³C NMR spectrum of 4',5-dihydroxy-6,7-(2,2-dimethylpyrano)-2'-methoxy-8- γ - γ -dimethylallflavone (1)



S5: EIMS spectrum of 4',5-dihydroxy-6,7-(2,2-dimethylpyrano)-2'-methoxy-8-γ-γ-dimethylallflavone (1)

Cudraflavone A (2) : Yellow needles (5.4 mg, 0.03%). R_f 0.45 (*n*-hexane: EtOAc = 4 :1),); IR (ATR) υ_{max} cm⁻¹: 3403 (OH), 2976 (sp^3 CH), 1649 (C=O), 1622 and 1561 (C=C aromatic), and 1208 (C-O); ¹H NMR (CD₃COCD₃, 400 MHz) δ ppm: 13.29 (s, 5-OH), 7.74 (1H, d, *J* = 8.4 Hz, H-5'), 6.68 (1H, d, *J* = 10.0 Hz, H-14), 6.64 (1H, dd, *J* = 8.4 Hz and 2.4 Hz, H-4'), 6.48 (1H, s, H-8), 6.44 (1H, d, *J* = 2.4 Hz, H-2'), 6.21 (1H, d, *J* = 9.2 Hz, H-10), 5.79 (1H, d, *J* = 10.0 Hz, H-15), 5.49 (1H, d, *J* = 9.2 Hz, H-9), 1.96 (3H, s, H-17), 1.70 (3H, s, H-18), 1.46 (6H, s, H-12 and H-13) ; ¹³C-NMR (CD₃COCD₃, 100 MHz) δ ppm: 178.3 (C-4), 163.4 (C-7), 159.0 (C-5), 158.2 (C-2), 156.4 (C-8a), 156.3 (C-3'), 155.8 (C-6'), 137.9 (C-11), 128.5 (C-15), 125.4 (C-5'), 121.2 (C-9), 114.9 (C-14), 110.1 (C-6'), 109.1 (C-4'), 107.4 (C-3), 105.2 (C-6), 105.2 (C-4a), 104.0 (C-2'), 94.9 (C-8), 77.8 (C-16), 69.4 (C-10), 27.4 (C-12 and C-13), 24.9 (C-18), 17.7 (C-17); EIMS *m/z* (% rel. int.): 418 ([M]⁺, C₂₅H₂₂O₆.



S6: IR spectrum of cudraflavone A (2)



S8: ¹H NMR spectrum of cudraflavone A (2) (Expansion)



S9: ¹³C NMR spectrum of cudraflavone A (2)



S10: EIMS spectrum of cudraflavone A (2)

Artocarpin (**3**): Orange powder (41.2 mg, 0.23%); R_f 0.43 (*n*-hexane: EtOAc = 3:2), IR (ATR) v_{max} cm⁻¹: 3365 (OH), 2958 (sp^3 CH), 1646 (C=O), 1615 and 1466 (C=C aromatic) and 1203 (C-O); ¹H-NMR (CD₃COCD₃, 400 MHz) δ ppm: 13.98 (1H, s, 5-OH), 8.84 (2H, s, 2'-OH/4'-OH), 7.24 (1H, d, J = 8.4 Hz, H-6'), 6.74 (1H, dd, J = 16.4 Hz and 7.2 Hz, H-15), 6.62 (2H, d, J = 16.4 Hz, H-14), 6.58 (1H, d, J = 2.4 Hz, H-3'), 6.57 (1H, s, H-8), 6.54 (1H, dd, J = 8.4 Hz and 2.4 Hz, H-5'), 5.13 (1H, t, J = 7.2 Hz, H-10), 3.98 (3H, s, 7-OCH₃), 3.14 (1H, d, J = 7.2 Hz, H-9), 2.45 (1H, m, H-16), 1.59 (3H, s, H-13), 1.45 (3H, s, H-12), 1.10 (6H, d, J = 6.4 Hz, H-17 and H-18); ¹³C-NMR (CD₃COCD₃, 100 MHz) δ ppm: 182.4 (C-4), 162.9 (C-7), 161.6 (C-2), 160.6 (C-5), 158.9 (C-4'), 156.6 (C-8a), 156.3 (C-2'), 141.3 (C-15), 131.4 (C-6'), 121.1 (C-10), 121.0 (C-3), 116.1 (C-14), 112.0 (C-1'), 108.9 (C-6), 107.2 (C-5'), 104.7 (C-4a), 102.9 (C-3'), 89.7 (C-8), 55.7 (7-OCH₃), 33.1 (C-16), 24.9 (C-12), 23.7 (C-9), 22.2 (C-17 and C-18), 16.7 (C-13); EIMS m/z(% rel. int.): 436 (100) ([M]⁺, C₂₆H₂₈O₆.



S11: IR spectrum of artocarpin (3)



S12: ¹H NMR spectrum of artocarpin (3)





S13: ¹H NMR spectrum of artocarpin (3) (Expansion)



S14: ¹³C NMR and DEPT spectrum of artocarpin (3)



S15: EIMS spectrum of artocarpin (3)

Cycloartobiloxanthone (4): Orange powder (7 mg, 0.04%) : R_f 0.5 (*n*-hexane: EtOAc = 3:2), IR (ATR) υ _{max} cm⁻¹: 3404 (OH), 2975 (sp^3 CH), 1622 (C=O); ¹H-NMR (CD₃COCD₃, 400 MHz) δ ppm: 13.41 (s, 5-OH), 6.95 (1H, d, J = 10.0 Hz, H-14), 6.43 (1H, s, H-3'), 6.16 (1H, s, H-6), 5.70 (1H, d, J = 10.0 Hz, H-15), 3.44 (1H, dd, J = 15.2 and 6.8 Hz, H-9b), 3.23 (1H, dd, J = 15.2 and 6.8 Hz, H-10), 2.40 (1H, t, J = 15.2 Hz, H-9a), 1.68 (3H, s, H-13), 1.48 (6H, s, H-17/18), 1.34 (3H, s, H-12); ¹³C-NMR (CD₃COCD₃, 100 MHz) δ ppm: 180.5 (C-4), 161.7 (C-7), 160.6 (C-2), 158.6 (C-5), 151.2 (C-8a), 150.6 (C-2'), 146.2 (C-4'), 137.0 (C-5'), 132.8 (C-6'), 126.9 (C-15), 115.0 (C-14), 111.8 (C-3), 104.5 (C-1'), 103.9 (C-4a), 100.9 (C-8), 99.0 (C-7), 92.8 (C-11), 77.8 (C-16), 46.6 (C-10), 31.3 (C-12), 27.5 (C-17 and C-18), 22.4 (C-13), 19.5 (C-9); EIMS m/z (% rel. int.): 434 [M]⁺, C₂₅H₂₂O₇.



S16: IR spectrum of cycloartobiloxanthone (4)



S18: ¹H NMR spectrum of cycloartobiloxanthone (4) (Expansion)



S19: ¹³C NMR and DEPT spectrum of cycloartobiloxanthone (4)



S20: EIMS spectrum of cycloartobiloxanthone (4)

Artonin E (**5**): Orange powder (5.3 mg, 0.07%) R_f 0.3 (*n*-Hex:EtOAc = 3:2); IR (ATR) υ_{max} cm⁻¹: 3393 (OH), 2943 (sp^3 CH), 1649 (C=O), 1622 and 1561 (C=C aromatic), and 1208 (C-O), (CD₃COCD₃, 400 MHz) δ ppm: 13.26 (s, 5-OH), 6.89 (1H, s, H-6'), 6.63 (1H, d, J = 10.0 Hz, H-14), 6.61 (1H, s, H-3'), 6.17 (1H, s, H-6), 5.69 (1H, d, J = 10.0 Hz, H-15), 5.14 (1H, t, J = 7.2 Hz, H-10), 3.15 (2H, d, J = 7.2 Hz H-9), 1.59 (3H, s, H-13), 1.48 (3H, s, H-12), 1.46 (6H, s, H-17 and 18); ¹³C-NMR (CD₃COCD₃, 100 MHz) δ ppm: 182.4 (C-4), 161.8 (C-5), 161.1 (C-2), 159.0 (C-7), 152.3 (C-8a), 148.8 (C-4'), 138.1 (C-5'), 131.4 (C-11), 127.1 (C-15), 121.5 (C-10), 120.7 (C-3), 116.1 (C-6'), 114.5 (C-14), 110.5 (C-1'), 104.7 (C-4a), 103.7 (C-3'), 100.7 (C-8), 98.7 (C-6), 77.8 (C-16), 27.3 (C-17 and C-18), 24.9 (C-12), 23.7 (C-9), 16.7 (C-13). EIMS m/z (% rel. int.): 436 [M]⁺, C₂₅H₂₄O₇.



S21 : IR spectrum of artonin E (5)







S24: EIMS spectrum of artonin E (5)

Oxyresveratrol (**6**) Yellow solid; (24.6 mg, 0.45%). R_f 0.38 (*n*-hexane:Et₂O = 2:3); IR (ATR) v_{max} cm⁻¹: 3209 (OH), 2921 (*sp*³ CH), 1589 (C=C aromatic); ¹H NMR (CD₃COCD₃, 400 MHz) δ ppm : 7.43 (1H, d, J = 8.4 Hz, H-6), 7.35 (1H, d, J = 16.4 Hz, H-β), 6.91 (1H, d, J = 16.4 Hz, H-α), 6.53 (1H, d, J = 2.0 Hz, H-2' and H- 6'), 6.45 (1H, d, J = 2.4 Hz, H-3), 6.39 (1H, dd, J = 8.4, 2.4 Hz, H-5), 6.24 (1H, t, J = 2.0 Hz, H-4'); ¹³C-NMR (CD₃COCD₃, 100 MHz) δ ppm : 158.7 (C-3',5'), 158.2 (C-2), 156.0 (C-4), 140.8 (C-1'), 127.4 (C-6), 125.5 (C-α), 123.5 (C-β), 116.4 (C1), 107.6 (C-5), 104.6 (C-2' and C-6'), 102.7 (C-3), 101.4 (C-4'). EIMS m/z (% rel. int.): 244 [M]⁺, C₁₄H₁₂O₄.



S25: IR spectrum of oxyresveratrol (6)



S27: ¹³C NMR spectrum of oxyresveratrol (6)



S28: EIMS spectrum of oxyresveratrol (6)

Macakurzin C (7): Yellow needle (3.3 mg, 0.07%); $R_f 0.38$ (*n*-hexane:EtOAc = 1:1); IR (ATR) v_{max} cm⁻¹: 3319 (OH), 2917 and 2847 (*sp*³ CH), 1652 (C=O) and 1584 (C=C aromatic); ¹H NMR (CDCl₃, 400 MHz) δ ppm: 12.21 (1H, s, 5-OH), 8.43 (1H, s, 3-OH), 8.32 (2H, d, *J* = 6.8 Hz, H-2' and H-6'), 7.56 (2H, t, *J* = 6.8 Hz, H-3' and H-5'), 7.55 (1H, d, *J* = 7.5 Hz, H-4'), 6.96 (1H, d, *J* = 10.0 Hz, H-9), 6.23 (1H, s, H-8), 5.80 (1H, d, *J* = 10.0 Hz, H-10), 1.50 (6H, s, H-12 and H-13); ¹³C NMR (CDCl₃, 100 MHz) δ ppm: 175.6 (C-4), 160.5 (C-7), 160.0 (C-9), 151.2 (C5), 144.8 (C-2), 136.6 (C-3), 130.9 (C-1'), 130.3 (C-4'), 128.9 (C-8'), 128.7 (C-3' and C-5'), 127.5 (C-2' and C-6'), 114.7 (C-7'), 103.8 (C-6), 101.44 (C-10), 99.8 (C-8), 78.3 (C-9'), 29.7 (C-10'), 28.2 (C-11'); EIMS m/z (% rel. int.): 336 [M]⁺ C₂₀H₁₆O₅).



S29: IR spectrum of macakurzin C (7)



S30: ¹H NMR spectrum of macakurzin C (7)



S31: ¹H NMR spectrum of macakurzin C (7) (Expansion)



S32: ¹³C NMR spectrum of macakurzin C (7)



S33: EIMS spectrum of macakurzin C (7)

Flemichapparin A (**8**): red solid (17.5 mg, 0.44 %); R_{*f*} 0.5 (*n*-hexane:EtOAc = 4:1); IR (ATR) ν_{max} cm⁻¹: 3242 (OH), 2917 (*sp*³ CH), 1594, 1465 (C=C aromatic); ¹H-NMR (CD₃COCD₃, 400 MHz) δ ppm : 14.13 (1H, s, 5-OH), 8.13 (1H, d, *J* = 16.0 Hz, H-β), 7.79 (1H, d, *J*=16.0 Hz, H-α), 7.41-7.64 (5H, m, H-2'-H-6'), δ 6.61 (1H, d, *J*=10.0 Hz, H-1"), 6.00 (1H, s, H-6), 5.52 (1H, d, *J*=10.0 Hz, H-2"), 1.58 (6H, s, H-4"/5"); ¹³C NMR (CD₃COCD₃, 100 MHz) δ ppm: 192.9 (C-1), 166.6 (C-3), 158.3 (C-7), 156.7 (C-5), 142.3 (C-α), 135.6 (C-1'), 130.9 (C-1'), 128.4 (C-3',C-4' and C-5'), 127.5 (C-2' and C-6'), 127.5 (C-β), 124.8 (C-2"), 106.6 (C-1"), 102.4 (C-4), 96.4 (C-6), 78.2 (C-3"), 28.1 (C-5"), 28.0 (C-4"); EIMS *m*/*z* (% rel. int.): 322 [M]⁺, C₂₀H₁₈O₄.



S33: IR spectrum of flemichapparin A (8)







S35: ¹H NMR spectrum of flemichapparin A (8) (Expansion)



S36: ¹³C NMR spectrum of flemichapparin A (8)



S37: EIMS spectrum of flemichapparin A (8)

Luteolin (**9**): yellow solid (13 mg, 0.13%) ; R_f 0.55 (*n*-hexane:EtOAc = 2:3); IR (ATR) v_{max} cm⁻¹: 3421 (OH), 2957, 2925 and 2632 (*sp*³ CH), 1653 (C=O), 1608 (C=C aromatic); ¹H NMR (CD₃COCD₃, 400 MHz) δ ppm: 13.05 (1H, s, 5-OH), 7.15 (1H, d, *J* = 2.4 Hz, H-2'), 7.49 (1H, dd, *J* = 8.4 Hz and 2.4 Hz, H-6'), 7.01 (1H, d, *J* = 8.4 Hz, H-5'), 6.60 (1H, s, H-3), 6.54 (1H, d, *J* = 2.0 Hz, H-6), 6.26 (1H, d, *J* = 2.0 Hz, H-8); ¹³C-NMR (CD₃COCD₃, 100 MHz) δ ppm: 182.1 (C-4), 164.3 (C-2), 164.1 (C-5), 162.5 (C-7), 157.9 (C-8a), 149.5 (C-3'), 145.7 (C-4'), 122.7 (C-1'), 119.2 (C-6'), 115.8 (C-5'), 113.2 (C-2'), 104.4 (C-4a), 103.3 (C-3), 98.8 (C-5), 93.8 (C-6). EIMS *m/z* (% rel. int.): 286 [M]⁺, C₁₅H₁₀O₆.



S38: IR spectrum of luteolin (9)



S40: ¹H NMR spectrum of luteolin (9) (Expansion)







S42: EIMS spectrum of luteolin (9)

Apigenin (10): yellow solid (5 mg, 0.05%); $R_f 0.45$ (*n*-hexane:EtOAc = 1:1); IR (ATR) υ_{max} cm⁻¹: 3426 (OH), 2962, 2920 and 2628 (*sp*³ CH), 1658 (C=O), 1608 (C=C aromatic); ¹H NMR (CD₃COCD₃, 400 MHz) δ ppm : 13.04 (1H, s, 5-OH), 7.96 (2H, d, *J* = 8.4 Hz, H-2' and H-6'), 7.04 (2H, d, *J* = 8.4 Hz, H-3' and H-5'), 6.65 (1H, s, H-3), 6.56 (1H, d, *J* = 2.0 Hz, H-6), 6.27 (1H, d, *J* = 2.0 Hz, H-8); ¹³C-NMR (CD₃COCD₃, 100 MHz) δ ppm : 182.2 (C-4), 164.2 (C-5), 164.0 (C-2), 162.5 (C-4'), 161.0 (C-9), 157.9 (C-7), 128.4 (C-2'/6'), 122.4 (C-1'), 115.9 (C-3'/5'), 104.5 (C-10), 103.2 (C-3), 98.8 (C-6), 93.8 (C-8); EIMS *m/z* (% rel. int.): 270 [M]⁺, C₁₅H₁₀O₅.



S43: IR spectrum of apigenin (10)



S45: ¹³C NMR spectrum of apigenin (10)



S46: EIMS spectrum of apigenin (10)

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