

SUPPORTING INFORMATION

Antiprotozoal Compounds from *Psorothamnus polydenius*

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List of supporting information:

1. **Figure S1.** ^1H NMR spectrum of 2,2',4'-trihydroxy-6'-methoxy-3',5'-dimethylchalcone (**2**).
2. **Figure S2.** ^{13}C NMR spectrum of 2,2',4'-trihydroxy-6'-methoxy-3',5'-dimethylchalcone (**2**).
3. Physical and spectral data for compounds **3-6**.

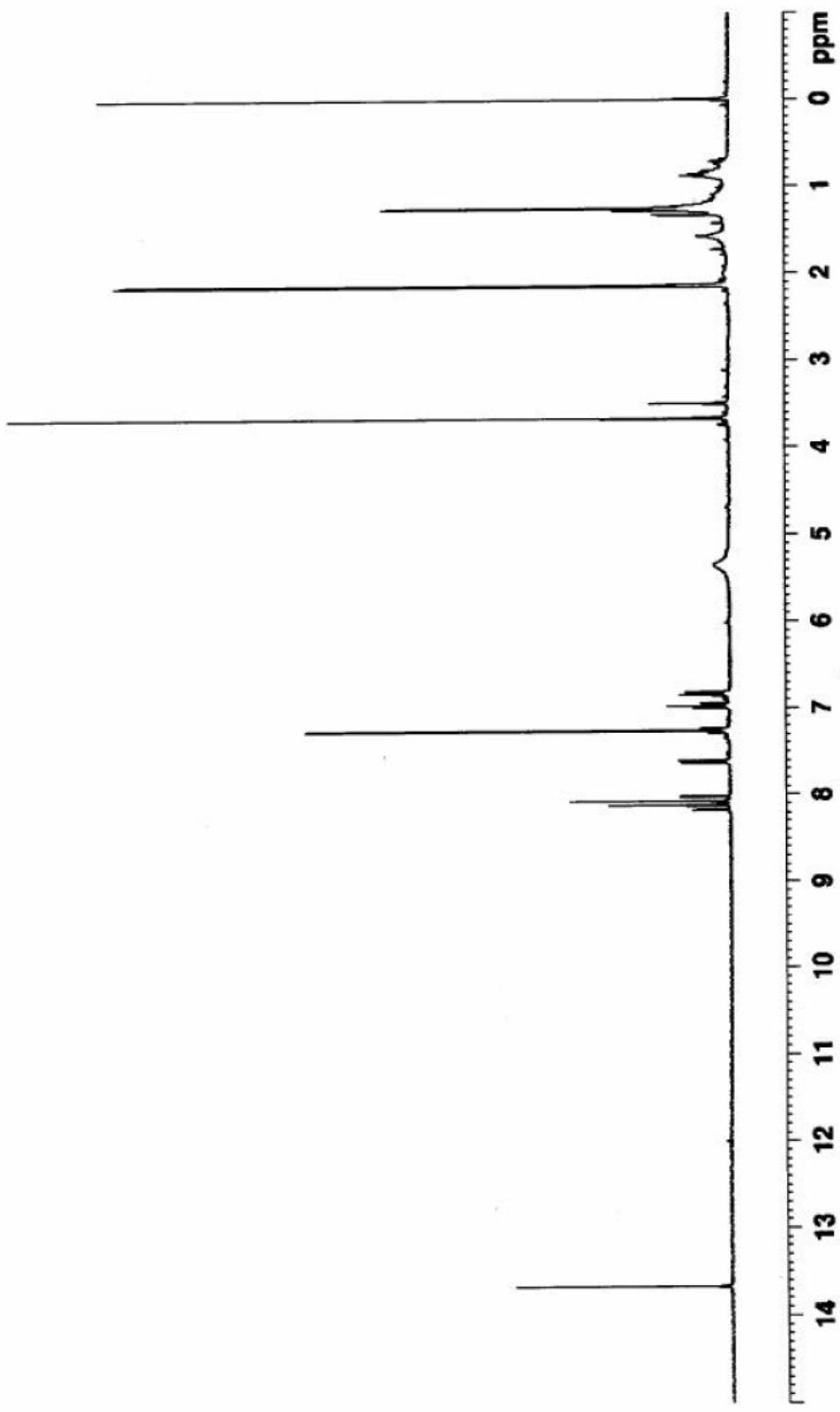


Figure S1. ¹H NMR spectrum of 2,2',4'-trihydroxy-3',5'-dimethylchalcone (**2**) in CDCl₃ (300 MHz NMR).

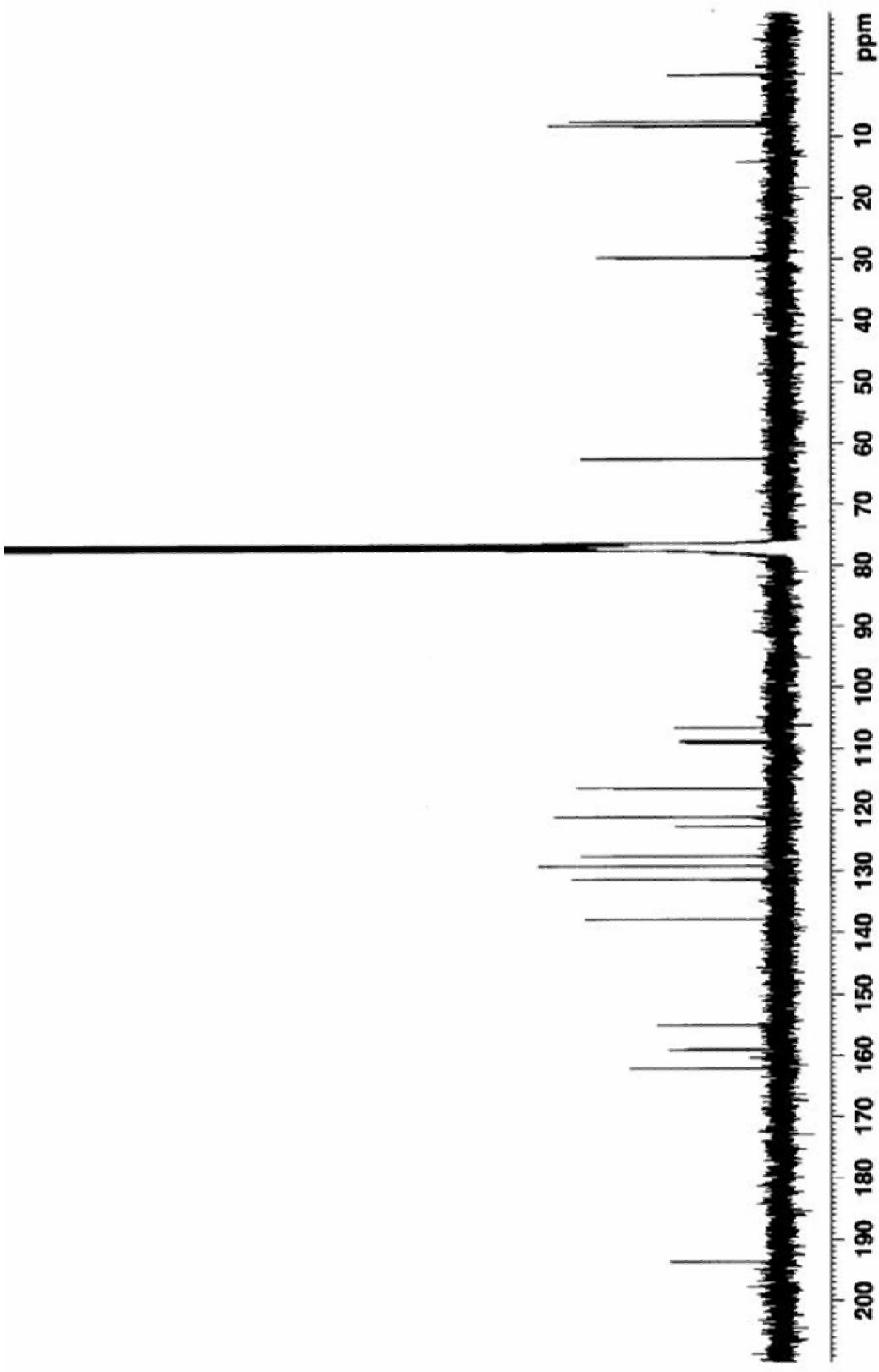


Figure S2. ¹³C NMR spectrum of 2,2',4-trihydroxy-6'-methoxy-3',5'-dimethylchalcone (**2**) in CDCl_3 (75 MHz NMR).

Dalrubone (3): Dark red plates, mp 99-100 °C (lit.⁸ 98-100 °C); UV, IR, and ¹H and ¹³C NMR data consistent with literature values;⁸ UV (MeOH) λ_{max} (log ε) 225 sh (4.28), 306 (3.85), 426 (4.09); IR ν_{max} (KBr) 3050, 2964, 2924, 2850, 1679, 1626, 1578, 1559, 1529, 1485, 1445, 1398, 1382, 1254, 1234, 1148, 1139, 1121 cm⁻¹; ¹H NMR (CDCl₃, 600 MHz) δ 7.70 (1H, d, *J* = 10.0, H-3), 7.44 (1H, ddd, *J* = 1.6, 7.5, 8.5, H-7), 7.32 (1H, dd, *J* = 1.6, 7.6, H-5), 7.27 (1H, d, *J* = 7.5, H-8) (the second *J* value corresponding to meta coupling with H-6 could not be obtained as the CDCl₃ peak lies in the same position), 7.21 (1H, ddd, *J* = 1.0, 7.6, 8.5, H-6), 7.17 (1H, d, *J* = 10.0, H-4), 3.82 (3H, s, OCH₃), 1.95 (3H, s, CH₃-5'), 1.34 (6H, s, CH₃-8', 9'); ¹³C NMR (CDCl₃, 150 MHz) δ 202.1 (C, C-2'), 199.4 (C, C-4'), 166.3 (C, C-6'), 156.5 (C, C-2), 152.7 (C, C-9), 133.5 (CH, C-4), 131.5 (CH, C-7), 127.3 (CH, C-5), 124.8 (CH, C-6), 120.8 (C, C-10), 119.4 (CH, C-3), 118.2 (C, C-5'), 116.2 (CH, C-8), 105.6 (C, C-1'), 59.5 (CH₃, OCH₃), 57.6 (C, C-3'), 23.0 (CH₃, C-8', 9'), 9.1 (CH₃, C-7').

Demethoxymatteucinol (6,8-dimethylpinocembrin) (4): Pale yellow needles, mp 201-202 °C (lit.⁶ 211 °C); [α]_D - 57.4 ° (c 0.5, MeOH at 24 °C); UV, IR, and ¹H and ¹³C NMR data consistent with literature values;⁶ the structure was confirmed by HSQC and HMBC spectroscopy; UV (MeOH) λ_{max} (log ε) 205 (4.55), 230 (sh 4.21), 297 (4.24), 345 (3.59); IR ν_{max} (KBr) 3235 (br OH), 1633, 1608, 1590, 1471, 1370, 1323, 1291, 1227, 1196, 1174, 1130, 1110 cm⁻¹; ¹H NMR (acetone-*d*₆, 600 MHz) δ 12.41 disappears on D₂O addition (1H, s, OH-5), 8.44 disappears on D₂O addition (1H, br s, OH-7), 7.58 (2H, d, *J* = 7.4 Hz, H-2' and H-6'), 7.45 (2H, dd, *J* = 7.4, 7.4 Hz, H-3' and H-5'), 7.39 (1H, dd, *J* = 7.4, 7.4 Hz, H-4'), 5.54 (1H, dd, *J* = 3.8, 12.7 Hz, H-2), 3.11 (1H, dd, *J* = 12.7, 17.0 Hz, H-3_{ax}), 2.85 (1H, dd, *J* = 3.8, 17 Hz, H-3_{eq}), 2.06 (3H, s, CH₃-8), 2.05 (3H, s,

$\text{CH}_3\text{-}6)$; ^{13}C NMR (acetone- d_6 , 150 MHz) δ 197.3 (C, C-4), 163.2 (C, C-7), 159.7 (C, C-5), 158.5 (C, C-9), 140.3 (C, C-1'), 129.4 (CH, C-3', 5'), 129.1 (CH, C-4'), 126.9 (CH, C-2', 6'), 104.3 (C, C-6), 103.5 (C, C-8), 102.9 (C, C-10), 79.4 (CH, C-2), 43.5 (CH_2 , C-3), 8.2 (CH_3 , C-8), 7.5 (CH_3 , C-6); EIMS m/z (rel. int. %) 284 [$\text{M}]^+$ (74), 207 [$\text{M-C}_6\text{H}_5]^+$ (37), 180 [$\text{M-C}_6\text{H}_5\text{-CH=CH}_2]^+$ (67), 152 [$\text{M-C}_6\text{H}_5\text{-CH=CH-CHO}]^+$ (100); HRESIMS m/z 307.0960 [$\text{M} + \text{Na}]^+$ (calcd for $\text{C}_{17}\text{H}_{16}\text{O}_4\text{Na}$, 307.0946).

Eriodictyol (5): White powder, mp 263-265 °C (dec., lit. 13 265-266 °C); $[\alpha]_D$ -21.5 ° (c 1.0, MeOH at 25 °C); UV, IR, and ^1H and ^{13}C NMR data consistent with literature values; 7,13 UV (MeOH) λ_{max} (log ϵ) 205 (4.85), 230 (sh 4.56), 287 (4.45), 330 (sh 3.82) nm; IR ν_{max} (KBr) 3355 (br OH), 1636, 1604, 1474, 1450, 1311, 1274, 1259, 1159 cm^{-1} ; ^1H NMR (methanol- d_4 , 300 MHz) δ 6.91 (1H, s, H-2'), 6.78 (2H, m, H-5' and H-6'), 5.89 (1H, d, J = 2.2 Hz, H-6), 5.88 (1H, d, J = 2.2 Hz, H-8), 5.27 (1H, dd, J = 3.1, 12.7 Hz, H-2), 3.06 (1H, dd, J = 12.7, 17.2 Hz, H-3_{ax}), 2.68 (1H, dd, J = 3.1, 17.2 Hz, H-3_{eq}); ^{13}C NMR (methanol- d_4 , 75 MHz) δ 197.9 (C, C-4), 168.5 (C, C-7)^a, 165.6 (C, C-5)^a, 162.0 (C, C-9)^a, 147.0 (C, C-3')^b, 146.6 (C, C-4')^b, 131.9 (C, C-1'), 119.4 (CH, C-6'), 116.4 (CH, C-5'), 114.9 (CH, C-2'), 103.5 (C, C-10), 97.3 (CH, C-8)^c, 96.3 (CH, C-6)^c, 80.6 (CH, C-2), 44.2 (CH_2 , C-3), (assignments with the superscripts a, b and c might be interchanged); HRESIMS found m/z 311.0522 [$\text{M} + \text{Na}]^+$, calcd for $\text{C}_{15}\text{H}_{12}\text{O}_6\text{Na}$ 311.0532.

Photodalrubone (6a and 6b): Dark yellow residue, ^1H and ^{13}C NMR data consistent with literature values;⁵ ^1H NMR (CDCl_3 , 600 MHz) δ 8.53 and 8.35 (1H each, d, J = 9.5, H-3), 7.95 and 7.95 (1H each, d, J = 9.5, H-4), 7.74 – 7.67 and 7.74 – 7.67 (2H each, m, H-7, 8), 7.614 and 7.607 (1H each, m, H-5), 7.475 and 7.462 (1H each, ddd, J =

2.0, 6.3, 8.3 or 1.5, 7.0, 8.1, respectively, H-6), 4.17 and 4.11 disappear on D₂O addition (1H each, s, OH), 2.28 and 2.26 (3H each, s, acetyl CH₃), 1.20, 1.18, 1.172, 1.166 (3H each, s, CH₃-3' or 4'); ¹³C NMR (CDCl₃, 150 MHz) δ 208.7, 207.8 (C, COCH₃), 203.1, 201.2 (C, C-5' or 2'), 198.2, 196.0 (C, C-2' or 5'), 165.9, 165.4 (C, C-2), 152.6 (C, C-9), 142.7, 142.5 (CH, C-4), 133.8, 133.7 (CH, C-7), 128.15, 128.10 (CH, C-5), 126.6, 126.5 (CH, C-6), 121.3, 121.2 (C, C-10), 118.3, 118.2 (CH, C-3), 118.0 (CH, C-8), 104.9, 104.2 (C, C-1'), 92.8, 92.7 (C, C-3' or 4'), 53.6, 53.0 (C, C-4' or 3'), 27.6, 27.4 (CH₃, COCH₃), 24.6, 24.2 (CH₃, C-3' or 4' methyl), 16.8 (CH₃, C-3' or 4' methyl); NOE: irradiation of the H-4 results in enhancement of the H-3 and the H-5. Irradiation of the δ 2.28 Me results in enhancement of the δ 4.11 OH and δ 1.18 Me while irradiation of the δ 2.26 Me results in enhancement of the δ 4.17 OH and δ 1.172 Me. HSQC shows that the ¹³C resonance of δ 1.166 methyl is δ 24.2 and that of δ 1.20 methyl is 24.6. HMBC shows a correlation between δ 4.17 OH and both δ 207.8 and 198.2 keto groups, also a correlation between δ 4.11 OH and both δ 208.7 and 196.0 keto groups. The four Me groups at δ 1.20–1.166 show a correlation to the adjacent δ 203.1 and 201.2 keto groups although there was not enough resolution to determine which methyls belong to what isomer; HRESIMS *m/z* 335.0909 [M + Na]⁺ (calcd for C₁₈H₁₆O₅Na, 335.0895).