

Antitumor Activity and Mechanism of Robustic Acid from *Dalbergia benthami* Prain via Computational Target Fishing

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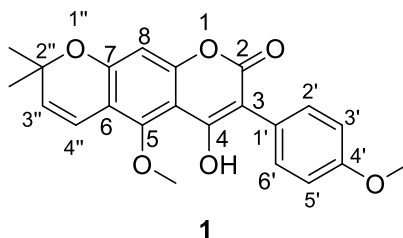
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Robustic acid: white solid, productivity: 40%; m.p. 208-20 °C; HR-MS(ESI) m/z : calculated for $C_{22}H_{20}O_6$ $[M + Na]^+$: 403.1157, found: 403.1157. 1H -NMR (400 MHz, $CDCl_3$) δ 9.97 (s, 1H, 4-OH), 7.46 (dd, 2H, J = 11.4 Hz, 2.9 Hz, H-2', H-6'), 6.97 (dd, 2H, J = 8.7 Hz, 2.9 Hz, H-3', H-5'), 6.63 (s, 1H, H-8), 6.50 (d, 1H, J = 10.0 Hz, H-4''), 5.77 (d, 1H, J = 10.0 Hz, H-3''), 3.96 (s, 3H, 4'-OCH₃), 3.77 (s, 3H, 5-OCH₃), 1.48 (s, 6H, -CH₃); ^{13}C -NMR (125 MHz, $CDCl_3$) δ 162.07 (C-4), 160.96 (C-2), 158.83 (C-4'), 157.97 (C-7), 153.65 (C-5), 152.11 (C-9), 131.78 (C-4''), 131.43 (C-2', 6'), 124.92 (C-6), 123.21 (C-1'), 115.03 (C-3''), 113.71 (C-3', 5'), 110.67 (C-8), 103.83 (C-10), 101.50 (C-3), 78.33 (C-2''), 65.19 (3'-OCH₃), 55.42 (5-OCH₃), 27.96 (2-2×CH₃).