

Antibacterial and cytotoxic activity of compounds isolated from

Flourensia oolepis

Mariana Belén Joray,¹ Lucas Daniel Trucco,² María Laura González,¹ Georgina Natalia Díaz Napal,¹ Sara María Palacios,¹ José Luis Bocco,² and María Cecilia Carpinella^{1*}

¹ *Fine Chemicals and Natural Products Laboratory, School of Chemistry, Catholic*

University of Córdoba, Avda Armada Argentina 3555, X5016DHK Córdoba, Argentina

² *CIBICI CONICET and Department of Clinical Biochemistry, Faculty of Chemical Science,*

National University of Córdoba, Haya de la Torre and Medina Allende, Córdoba, Argentina

Supplementary Material

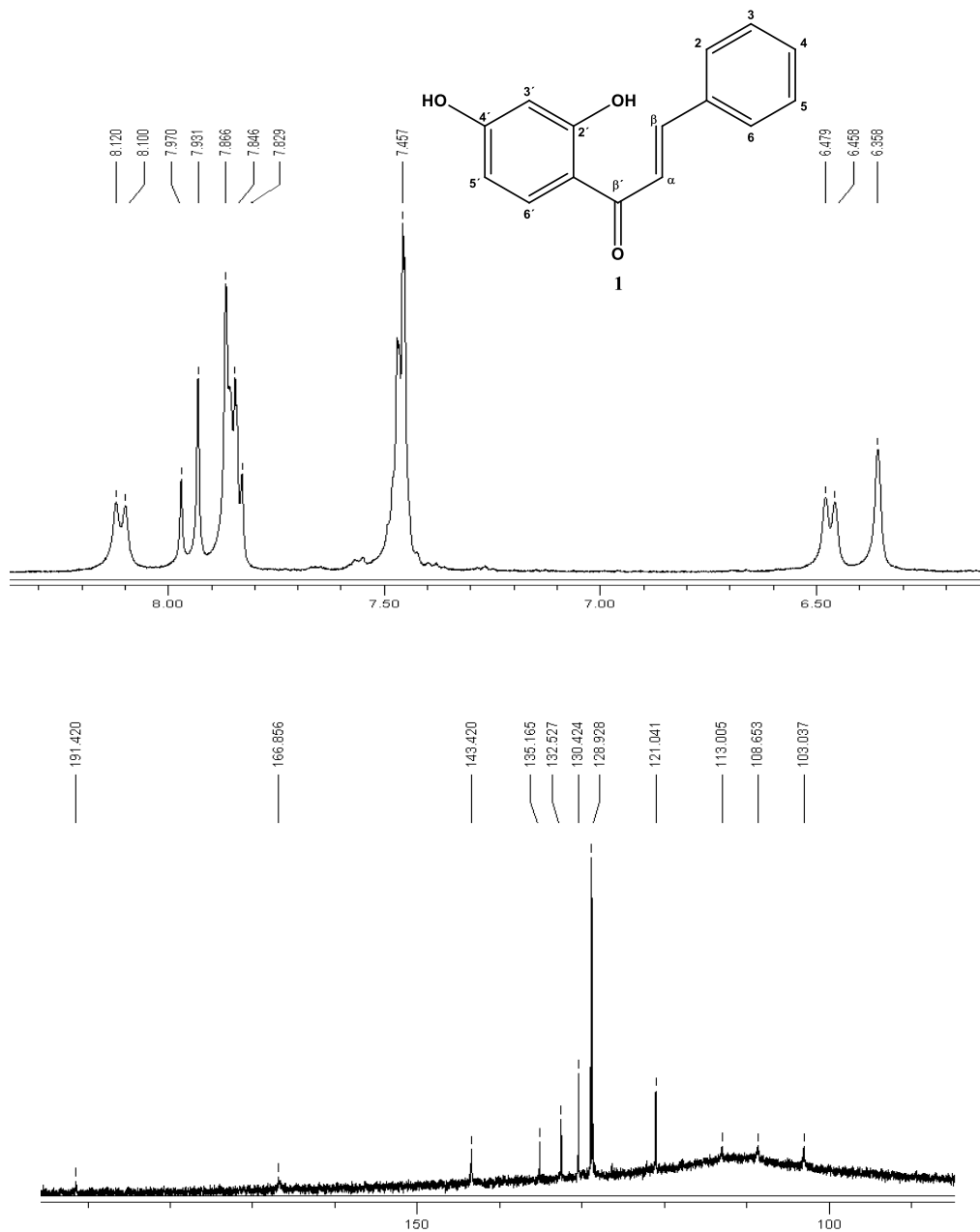


Figure 1. NMR spectra of 2',4'-dihydroxychalcone (**1**). ¹H NMR (400 MHz, CD₆O): δ (ppm) 8.11 (1 H, d, *J*=8.0 Hz, H-6'), 7.95 (1 H, d, *J*=15.6 Hz, H-α), 7.85 (1 H, d, *J*=14.8 Hz, H-β), 7.85-7.45 (5 H, m, H-2-6), 6.47 (1 H, d, *J*=8.4 Hz, H-5'), 6.35 (1 H, s, H-3'). ¹³C NMR (50 MHz, CD₆O): δ (ppm) 103.0 (C-3'); 108.6 (C-5'); 113.0 (C-1'); 121.0 (C-α); 128.9 (C-2,3,5,6); 130.4 (C-4); 132.5 (C-6'); 135.2 (C-1); 143.4 (C-β); 166.8 (C-2',4'); 191.4 (C=O).

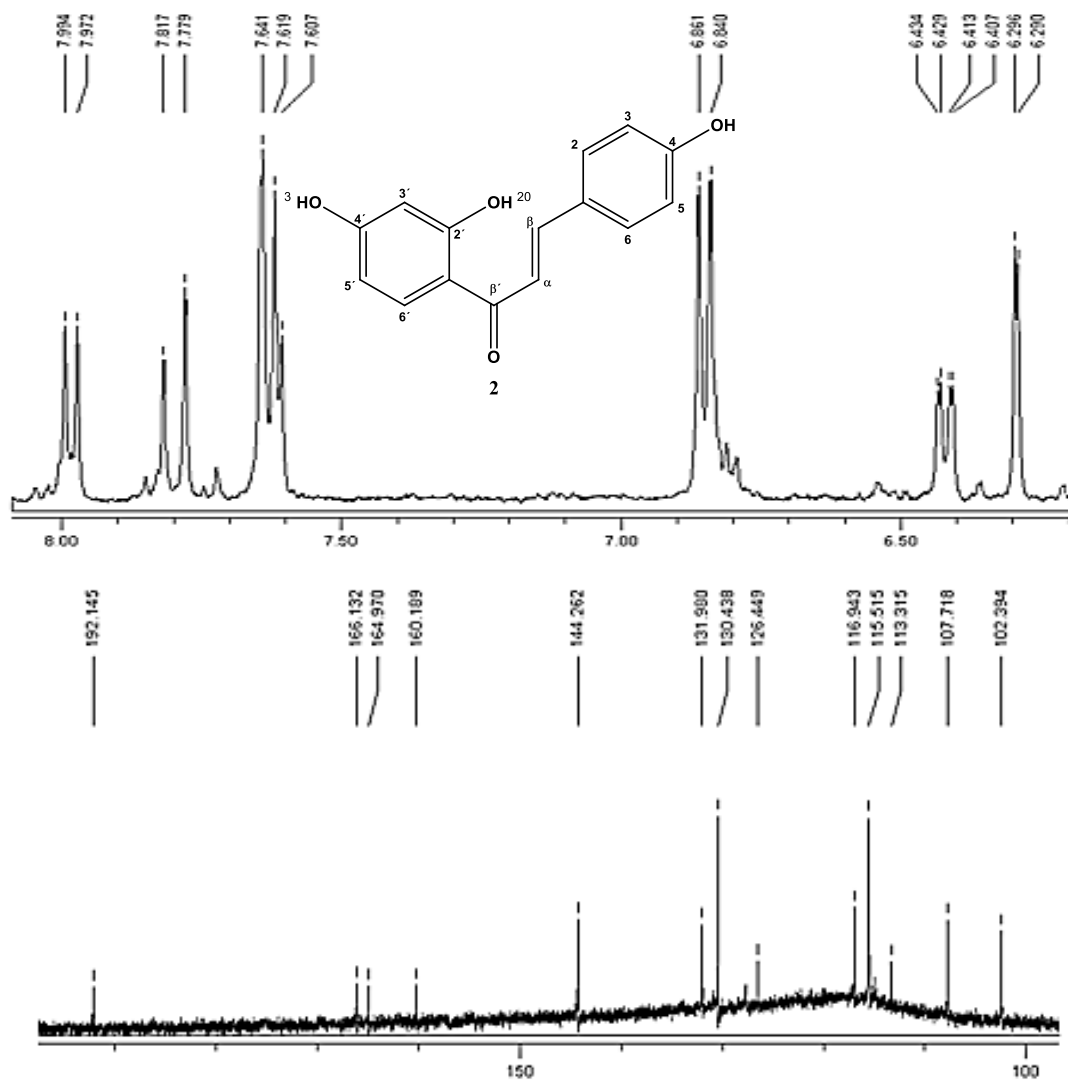


Figure 2. NMR spectra of isoliquiritigenin (**2**). ^1H NMR (400 MHz, CD_6O): δ (ppm) 7.96 (1 H, d, $J = 8.8$ Hz, H-2'), 7.79 (1 H, d, $J = 15.2$ Hz, H- β), 7.63 (2 H, d, $J = 9.2$ Hz, H-2, H-6), 7.62 (1 H, d, $J = 14.8$ Hz, H- α), 6.85 (2 H, d, $J = 8.8$ Hz, H-3, H-5), 6.42 (1 H, dd, $J = 8.8, 2.4$ Hz, H-3'), 6.29 (1 H, d, $J = 2.4$ Hz, H-5'). ^{13}C NMR (50 MHz, CD_6O): δ (ppm) 102.4 (C-5'), 107.7 (C-3'), 113.3 (C-1'), 115.2 (C-3, 5), 116.9 (C- α), 126.4 (C-1), 130.4 (C-2, 6), 131.9 (C-2'), 144.3 (C- β), 160.2 (C-4), 164.9 (C-4'), 166.1 (C-6'), 192.1 (C=O).

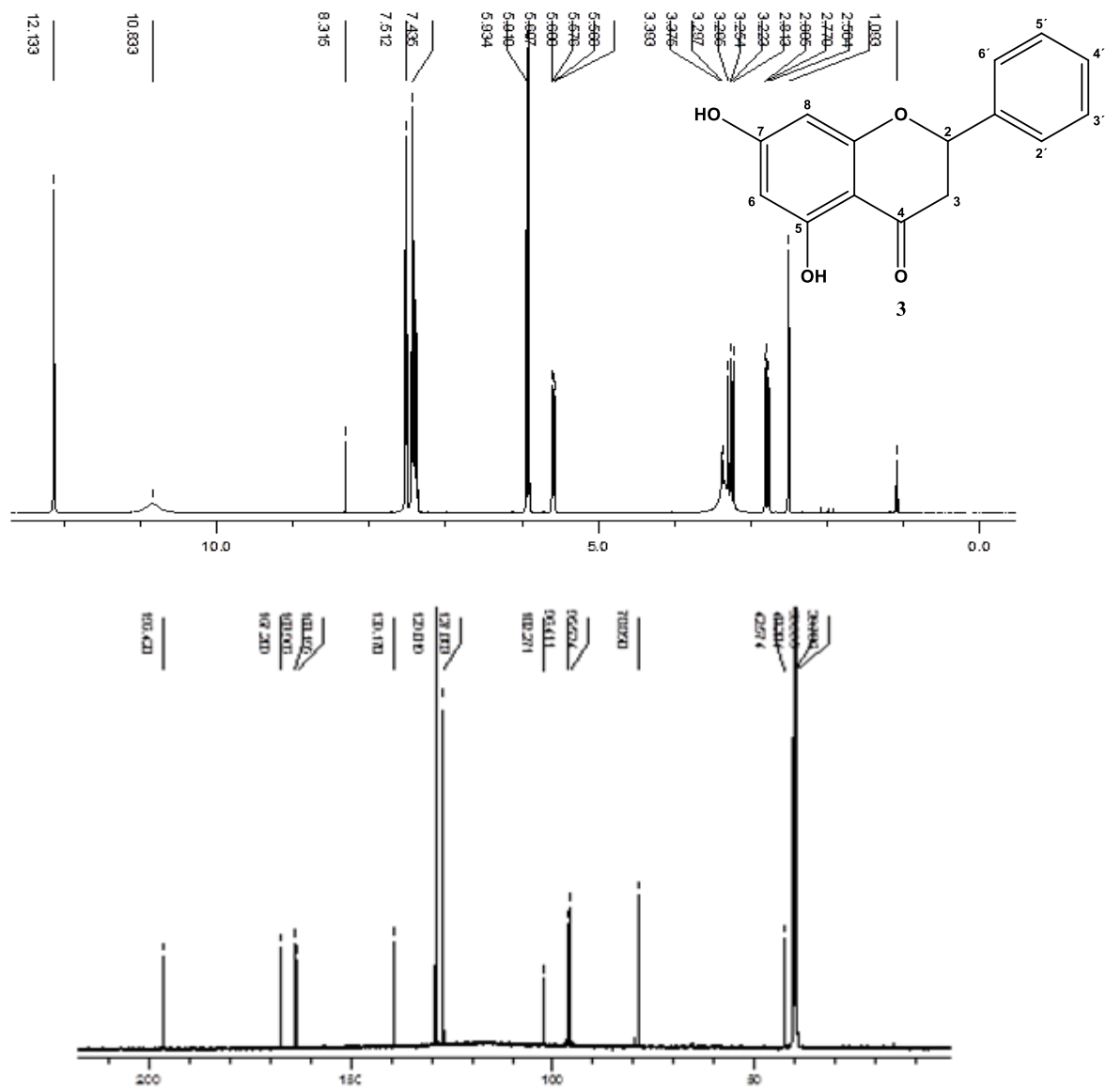


Figure 3. NMR spectra of pinocembrin (**3**). ¹H NMR (400 MHz, DMSO-d₆): δ (ppm) 7.41 (5H, m, H-20-60), 6.01 (1H, d, *J* = 2.2 Hz, H-8), 5.52 (1H, d, *J* = 2.2 Hz, H-6), 5.44 (1H, dd, *J* = 12.8, 3.2 Hz, H-2), 3.06 (1H, dd, *J* = 12.8, 17.2 Hz, H-3ax), 2.77 (1H, dd, *J* = 17.2, 3.2 Hz, H-3eq). ¹³C NMR (50 MHz, DMSO-d₆): δ (ppm) 40.4 (C-3), 80.2 (C-2), 95.9 (C-8), 96.8 (C-6), 102.7 (C-10), 127.5 (C-20/60), 129.4 (C-40) 129.5 (C-30/50), 139.6 (C-10), 163.6 (C-9), 164.4 (C-5), 167.6 (C-7), 196.7 (C-4).

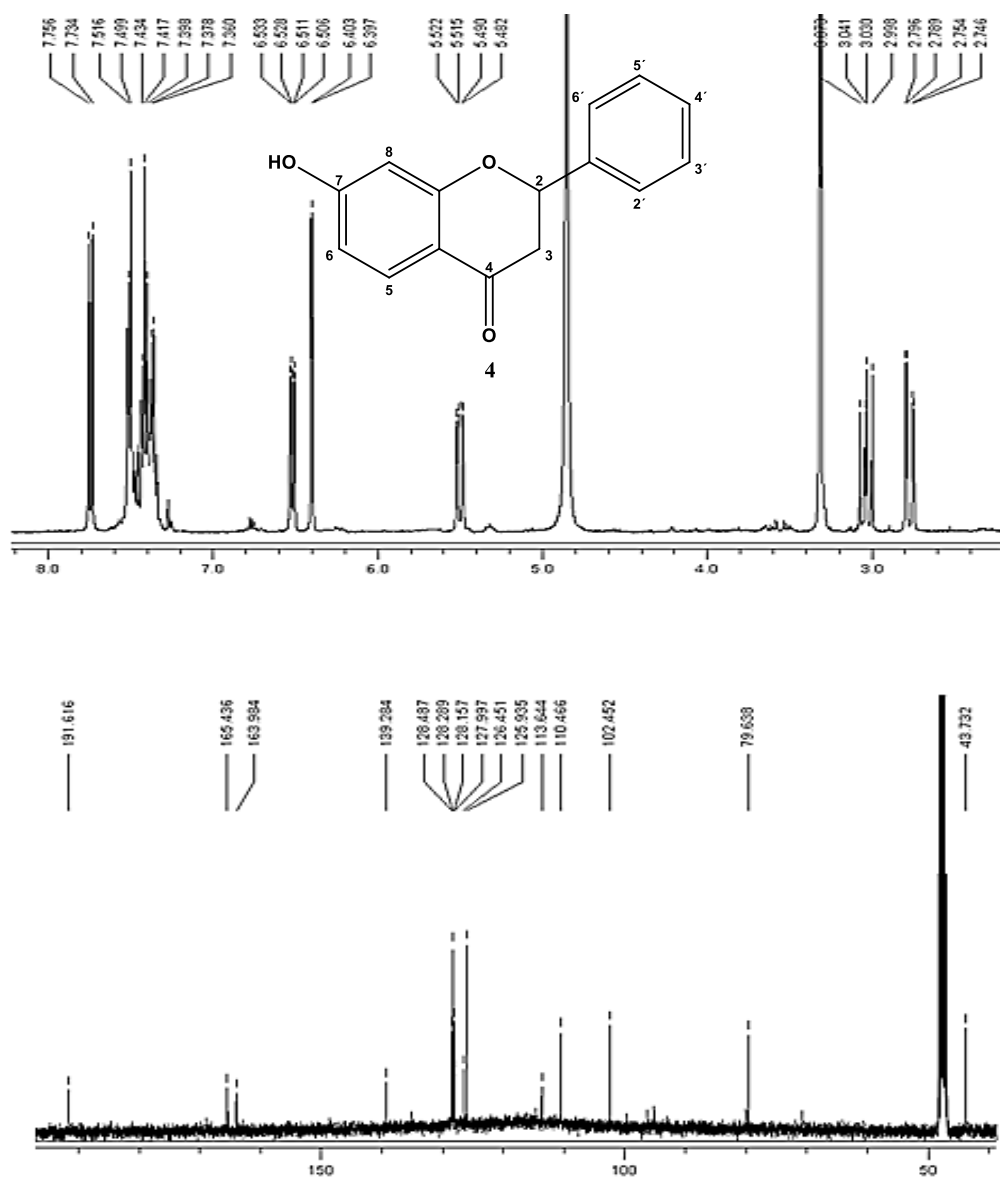


Figure 4. NMR spectra of 7-hydroxyflavanone (**4**). ^1H NMR (400 MHz, CD_6O): δ (ppm) 7.74 (1 H, d, $J = 8.8$ Hz, H-5), 7.50 (2 H, d, $J = 6.8$ Hz, H-2', H-6'), 7.42 (2 H, t, $J = 7.2$ Hz, H-3', H-5'), 7.36 (1 H, t, $J = 7.2$ Hz, H-4'), 6.52 (1 H, dd, $J = 8.8, 2.0$ Hz, H-6), 6.40 (1 H, d, $J = 2.4$ Hz, H-8), 5.50 (1 H, dd, $J = 12.8, 2.8$ Hz, H-2), 3.03 (1 H, dd, $J = 17.2, 12.8$ Hz, H-3ax), 2.79 (1 H, dd, $J = 16.8, 3.0$ Hz, H-3eq). ^{13}C NMR (50 MHz, CD_6O): δ (ppm) 43.7 (C-3), 79.6 (C-2), 102.4 (C-8), 110.5 (C-6), 113.4 (C-10), 125.9 (C-2'), 126.4 (C-6'), 128 (C-4'), 128.2 (C-3'), 128.3 (C-5'), 128.4 (C-5), 139.3 (C-1'), 163.3 (C-7), 165.4 (C-9), 191.6 (C=O).

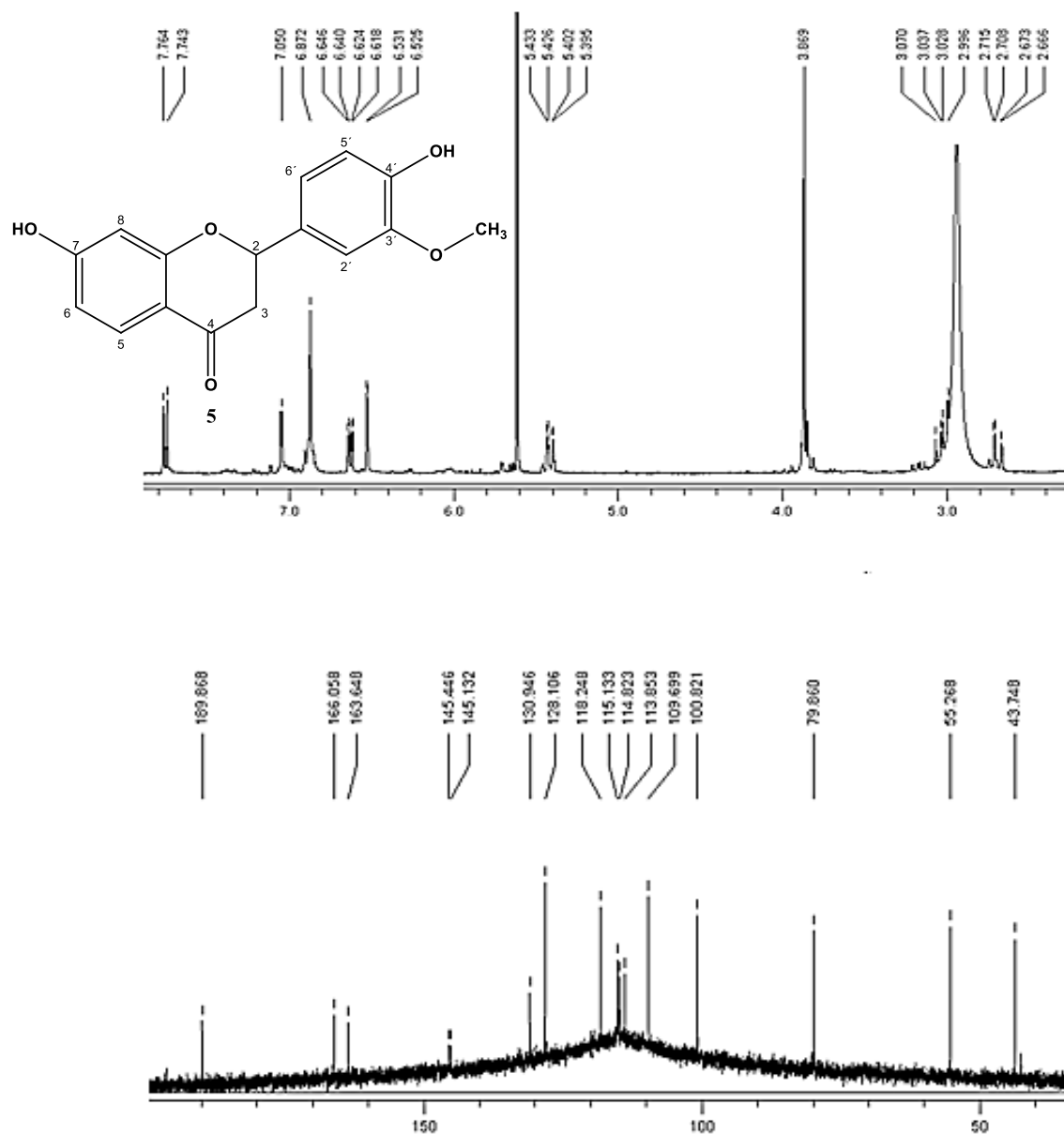


Figure 5. NMR spectra of 7,4'-dihydroxy-3'-methoxyflavanone (**5**). ^1H NMR (400 MHz, CD_6O): δ (ppm) 7.75 (1 H, d, $J = 8.4$ Hz, H-5), 7.05 (1 H, s, H-2'), 6.88 (1 H, d, $J = 7.6$ Hz, H-5'), 6.88 (1 H, dd, $J = 12.8, 5.2$ Hz, H-6'), 6.64 (1 H, dd, $J = 9.2, 2.8$ Hz, H-6), 6.53 (1 H, d, $J = 2.4$ Hz, H-8), 5.41 (1 H, dd, $J = 12.4, 2.8$ Hz, H-2), 3.87 (3 H, s, O- CH_3), 3.03 (1 H, dd, $J = 16.6, 12.8$ Hz, H-3 $_{\text{ax}}$), 2.69 (1 H, dd, $J = 16.8, 2.8$ Hz, H-3 $_{\text{eq}}$). ^{13}C NMR (50 MHz, CD_6O): δ (ppm) 43.8 (C-3), 55.3 (O- CH_3), 79.8 (C-2), 100.8 (C-8), 109.7 (C-6), 113.8 (C-2'), 114.8 (C-10), 115.1 (C-5'), 118.2 (C-6'), 128.1 (C-5), 130.9 (C-1'), 145.1 (C-4'), 145.4 (C-3'), 163.6 (C-9), 166.0 (C-7), 189.9 (C=O).