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J. Serb. Chem. Soc. 90 (3) S85–S90 (2025) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

Phytochemical investigation from wood residues of *Dalbergia spruceana* Benth

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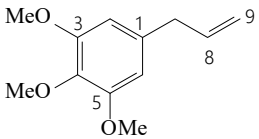
EXTRACTION AND ISOLATION OF COMPOUNDS

The wood residues of *Dalbergia spruceana* were submitted to maceration for 7 days with hexane and methanol, which provided yields of 0.05 and 3.67%, respectively. The fractionation of the methanol extract (19 g) was carried out on a silica gel column (70-230 mesh; h x ø = 30 x 5 cm), eluted with hexane-EtOAc (2-40%), and generated ninety fractions. Fr. 27 (47 mg) showed a predominance of β-sitosterol and stigmasterol. Fr. 46 (20 mg) was obtained by preparative thin layer chromatography (PTLC) eluted with CH_2Cl_2-acetone (98:2) and resulted in the purification of compound **1** (10 mg). Fr. 50 gave the solid compound **2** (900 mg). Fr. 61 (70.0 mg) was fractionated over a silica gel column (230-400 mesh; h x ø = 46 x 2.6 cm) and eluted with CH_2Cl_2. Subfractions 15 and 17 were submitted to new fractioning. Subfraction 15 (23.0 mg) was fractionated over silica gel column (230-400 mesh; h x ø = 38.5 x 1.2 cm) and eluted with CH_2Cl_2-MeOH (98:2) to obtain compound **3** (3.5 mg). Subfr. 17 (35 mg) resulted the isolation of compound **4** (5.5 mg), after purification in PTLC and elution with of CH_2Cl_2-MeOH (98:2). The fractionation of 71 (52.0 mg) over a silica gel column (230-400 mesh; h x ø = 37.0 x 2.6 cm) and elution with CH_2Cl_2-acetone (98:2) provided compound **5** (10.0 mg). The fraction 73 (80 mg) was fractionated over a silica gel column (230-400 mesh; h x ø = 8.0 x 0.7 cm), eluted with CH_2Cl_2-acetone (98:2) and resulted in the purification of **6** (3.5 mg). The fraction 83 gave the solid compound **7** (5.8 mg).

CHARACTERIZATION DATA FOR COMPOUNDS **1-3** AND **5-7**



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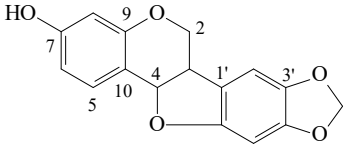
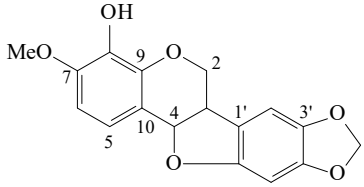
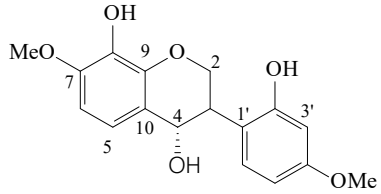
*Elemycin (**1**).* ^{1}H NMR (300 MHz, $CDCl_3$, J/Hz): 6.43 (s, H-2 and H-6), 5.97 (m, H-8), 5.11 (m, H-9), 3.87 (s, OC**H**$_3$-3 and 5), 3.84 (s, OC**H**$_3$-4), 3.36 (d, J = 6.7 Hz, H-7). ^{13}C NMR (75 MHz, $CDCl_3$): 153.1 (C-3 and C-5), 137.2 (C-8), 136.2 (C-4), 135.8 (C-1), 116.0 (C-9), 105.4 (C-2 and C-6), 60.8 (O**C**H$_3$-4), 56.0 (O**C**H$_3$-3 and 5), 40.55 (C-7).



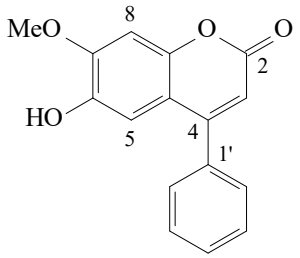
*Maackiain (**2**).* White solid. ^{1}H NMR (300 MHz, $(CD_3)_2CO$, J/Hz): 8.64 (s, OH), 7.31 (d, J = 8.3 Hz, H-5), 6.90 (s, H-2'), 6.57 (dd, J = 8.3 and 2.3 Hz, H-6), 6.40 (s, H-5'), 6.36 (d, J = 2.3 Hz, H-8), 5.93 and 5.91 (s, CH_2O_2), 5.50 (d, J = 6.5 Hz, H-4), 4.29 (dd, J = 10.5 and 3.9 Hz, H-2), 3.65 (t, J = 9.9 Hz, H-2), 3.57 (m, H-3). ^{13}C NMR (75 MHz, $(CD_3)_2CO$: 158.8 (C-7), 156.7 (C-9), 154.4 (C-6'), 147.9 (C-4'), 141.5 (C-3'), 132.1 (C-5), 118.6 (C-1'), 111.8 (C-10), 109.5 (C-6), 105.0 (C-2'), 103.0 (C-8), 101.2 (C-3'and C-4'), 93.0 (C-5'), 78.4 (C-4), 66.0 (C-2), 40.1 (C-3). ESI-MS m/z 283.0661 $[M-H]^-$.



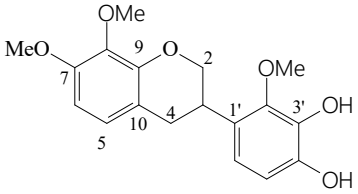
*8-hydroxy-7-methoxy-3',4'-methylenodioxypterocarpan (**3**).* White solid. ^{1}H NMR (300 MHz, $CDCl_3$, J/Hz): 7.06 (d, J = 8.6 Hz, H-5), 6.74 (s, H-5'), 6.69 (d, 8.6 Hz, H-6), 6.44 (s, H-2'), 5.94 and 5.91 (s, CH_2O_2), 5.54 (d, J = 7.0 Hz, H-4), 4.38 (dd, J = 10.8 and 3.9 Hz, H-2), 3.74 (t, J = 10.8 Hz, H-2), 3.57 (m, H-3). ^{13}C NMR (75 MHz, $CDCl_3$): 154.2 (C-6'), 148.1 (C-4'), 147.3 (C-7), 143.3 (C-9), 141.7 (C-3'), 133.9 (C-8), 121.0 (C-5), 117.6 (C-1'), 113.9 (C-10), 105.0 (C-6), 104.7 (C-2'), 101.3 (C-3'and C-4'), 93.8 (C-5'), 78.3 (C-4), 66.8 (C-2), 56.3 (MeO), 40.2 (C-3). ESI-MS m/z 313.0730 $[M-H]^-$.



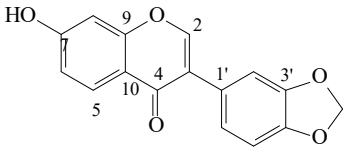
8,4,2' trihydroxy-7,4'-dimethoxyisoflavonol (**4**). Yellow amorphous solid. ^{1}H, ^{13}C NMR, NOESY, HSQC and HMBC (see the spectra below). ESI-MS 341.0994 $[M+Na]^+$.



*Dalbergin (**5**)*. Yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$, J/Hz): 7.52 (m, H-3', H-4'and H-5'), 7.52 (m, H-4'), 7.45 (m, H-2' and H-6'), 7.01(s, H-5), 6.92 (s, H-8), 6.27 (s, H-3), 4.01 (MeO-7). ^{13}C NMR (125 MHz, $CDCl_3$): 161.4 (C-2), 155.7 (C-4), 150.1 (C-7), 149.3 (C-9), 142.5 (C-6), 135.6 (C-1'), 129.5 (4'), 128.8 (C-3', C-5'), 128.3 (C-2', C-6'), 112.5 (C-3), 112.3 (C-10), 110.5 (C-5), 99.6 (C-8), 56.4 (MeO-7). ESI-MS m/z 267.0666 $[M+H]^+$.



*3',4'-Dihydroxy-7,8,2'-trimethoxyisoflavan (**6**)*. Whith solid. ^{1}H NMR (500 MHz, $CDCl_3$, J/Hz): 6.73 (d, J = 8.3 Hz, H-5), 6.67 (d, J =8.5 Hz, H-5'), 6.63 (d, J =8.5 Hz, H-6'), 6.55 d (d, J = 8.3 Hz, H-6), 4.42 (m, H-2a), 4.03 (t, J =10.3 Hz, H-2b), 3.94 (s, O**C**$\mathbf{H_3}$-8), 3.92 (s, O**C**$\mathbf{H_3}$-2'), 3.91 (s, O**C**$\mathbf{H_3}$-7), 3.59 (m, H-3), 2.95 (m, H-4b), 2.92 (m, H-4a). ^{13}C NMR (125 MHz, $CDCl_3$): 145.7 (C-2'), 147.5 (C-7 and C-9), 139.2 (C-4'), 138.7 (C-3'), 134.9 (C-8), 127.2 (C-1'), 124.2 (C-5), 116.9 (C-6'), 115.3 (C-10), 107.0 (C-6), 106.4 (C-5'), 70.5 (C-2), 61.0 (O**C**H_3-8), 60.9 (O**C**H_3-2'), 56.2 (O**C**H_3-7), 31.6 (C-3), 31.5 (C-4). ESIMS m/z 333.1313 $[M+H]^+$.



Pseudobaptigenin (**7**). White solid. ^{1}H NMR (500 MHz, C_5D_5N, J/Hz): 8.46 (d, J = 8.7Hz, H-5), 8.19 (s, H-2), 7.49 (d, J = 1.5 Hz, H-2'), 7.26 (dd, J = 8.7 and 2.3 Hz, H-6), 7.25 (d, J = 8.0 Hz, H-5'), 7.15 (d, J = 2.3 Hz, H-8), 7.0 (dd, J = 8.0 and 1.5 Hz , H-6'), 6.00 (s, CH_2O_2). ^{13}C NMR (125 MHz, C_5D_5N): 75.2 (C-4),163.9 (C-7), 158.3 (C-9), 152.7 (C-2), 147.8 (C-3'), 147.6 (C-4'), 127.9 (C-5), 126.6 (C-3), 124.3 (C-1'), 122.6 (C-5'), 117.5 (C-10), 115.7 (C-6), 110.1 (C-2'), 108.8 (C-6'), 102.8 (C-8), 101.4 (C-3',4').

SPECTRA OF THE NEW COMPOUND **4**

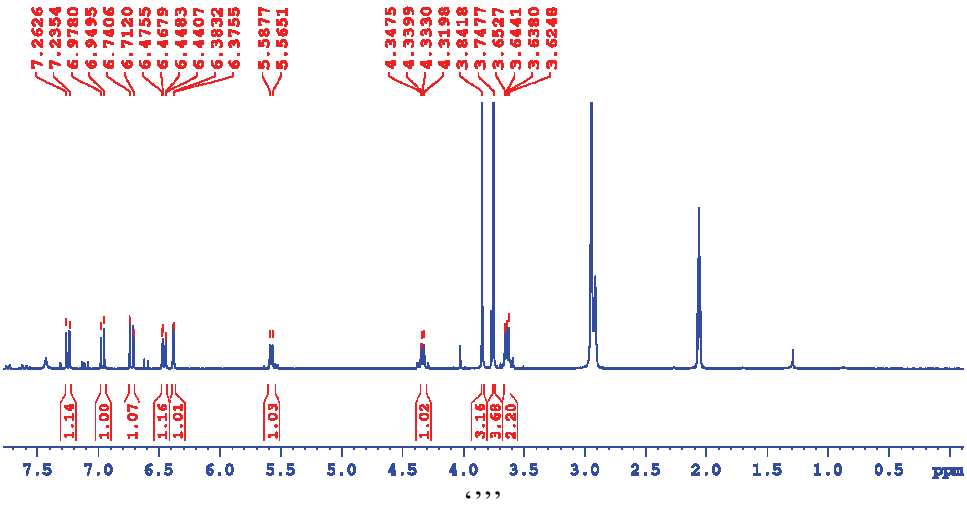


Figure S-1. ^{1}H-NMR spectrum of compound **4**

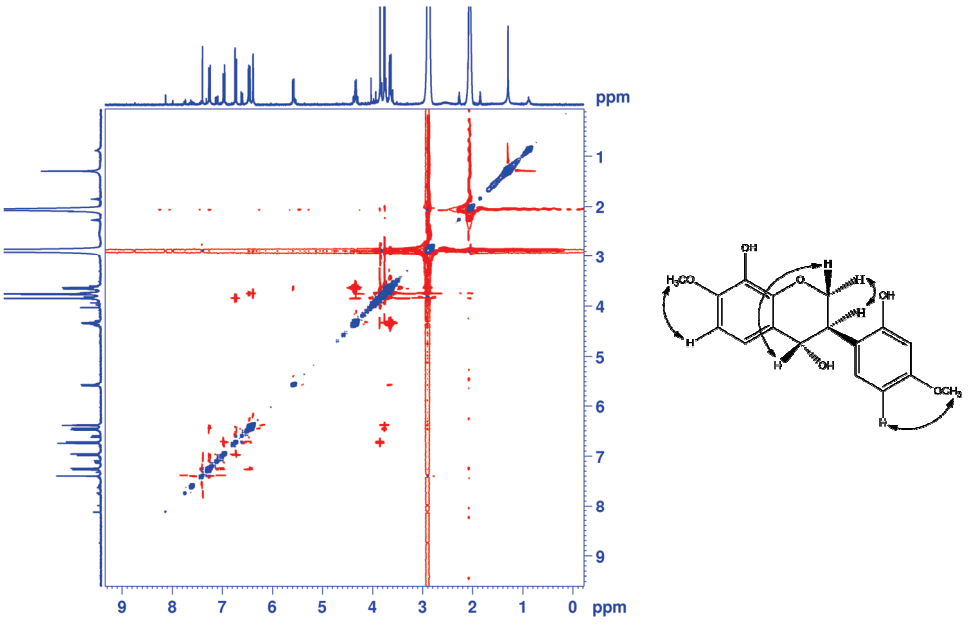


Figure S-2 NOESY spectrum of compound **4**

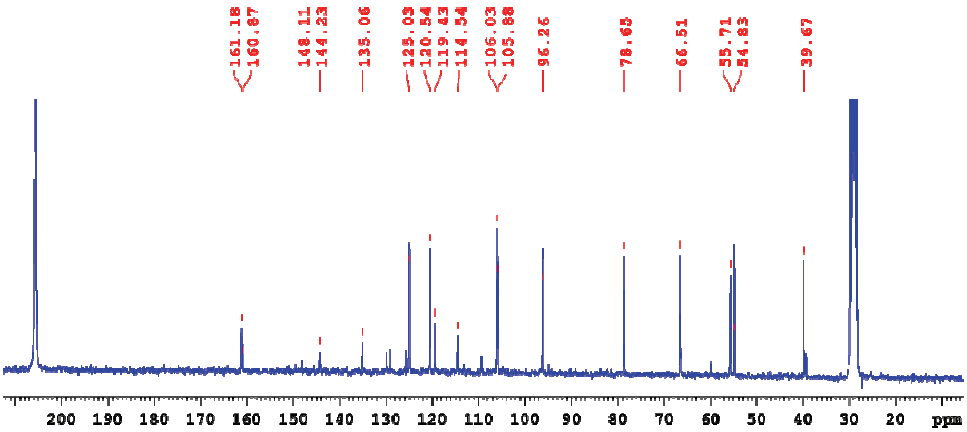


Figure S-3. ^{13}C RMN of compound **4**

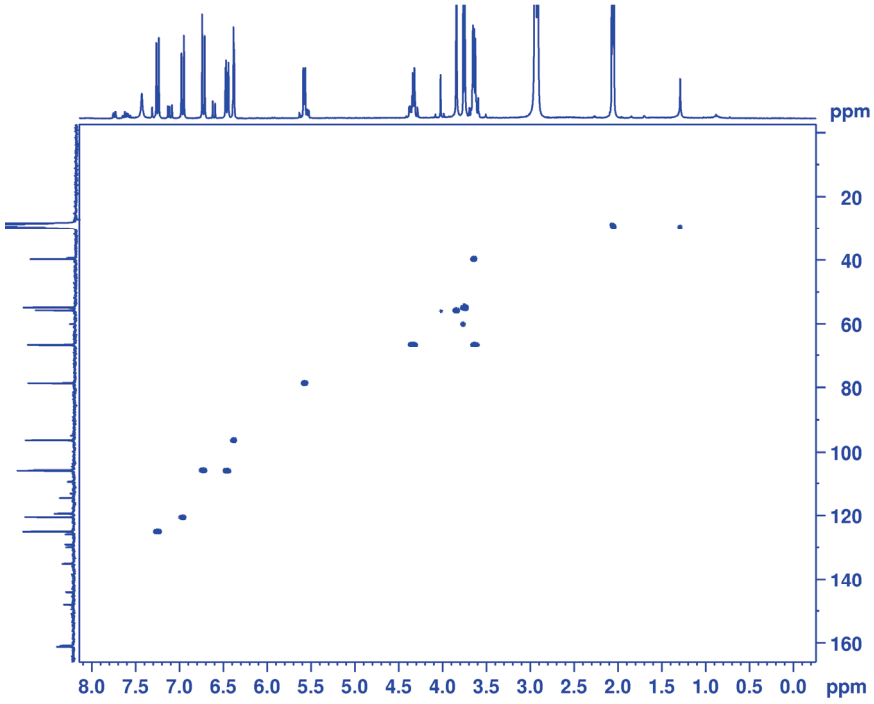


Figure S-4. HSQC spectrum of compound **4**.

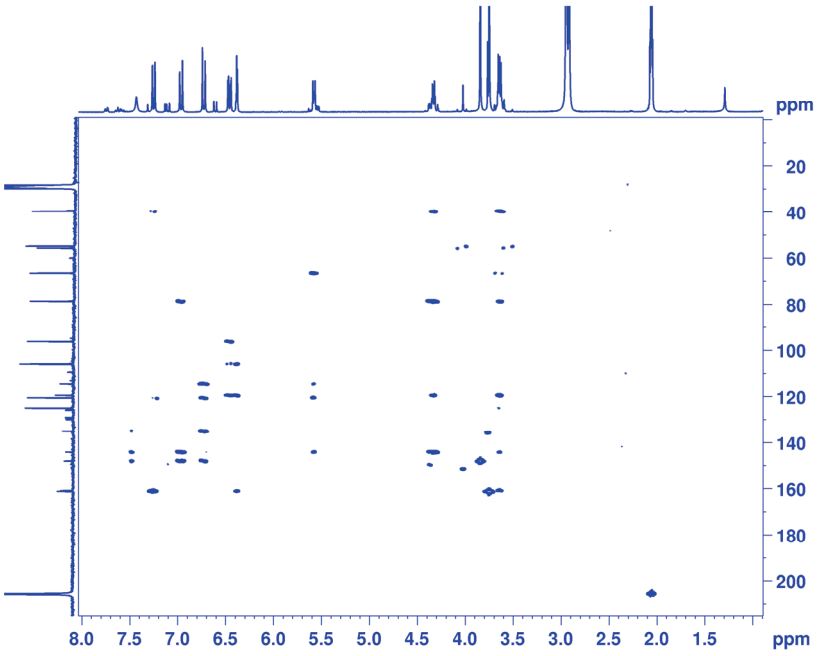


Figure S-5. HMBC spectrum ([300 MHz, 75 MHz $(CD_3)_2CO$]) of compound **4**.

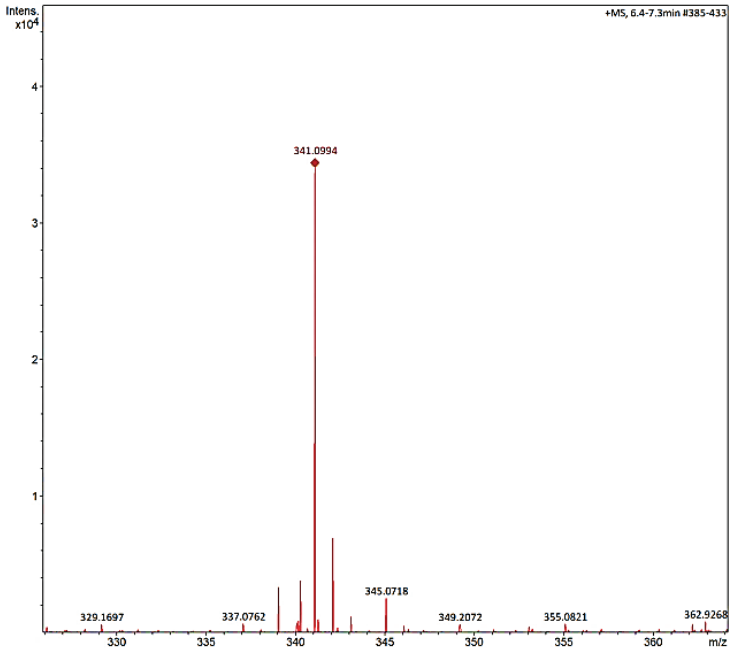


Figure S-6. HR-ESIMS spectrum of compound **4**.