CANDIDIN. A PYRANOFLAVONE FROM TEPHROSIA CANDIDA SEEDS

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In continuation [1] of our work on the seeds of Tephrosia candida, we report the isolation of a new flavone, candidin (1). It analysed for C₂₁H₁₈O₄ and did not give a ferric reaction, which suggested that the molecule did not contain a chelated phenolic hydroxyl group. The fact that candidin is a flavone was shown by absorption at $1630\,\mathrm{cm}^{-1}$ in the IR spectrum, $\lambda_{\mathrm{max}}^{\mathrm{MeOH}}$ 235, 270 and 345 nm in the UV spectrum and by a singlet at δ 6.3 (H-3) in the 1 H NMR spectrum [2]. A singlet at δ 7.60 integrating for five protons indicated the B-ring to be unsubstituted. A six-proton singlet at δ 1.50, assignable to a gem-dimethyl group, and two doublets ($J = 10 \,\mathrm{Hz}$) at $\delta 5.58$ and 6.80, each integrating for one proton, corresponding to vinylic protons (H-3" and H-4", respectively), suggested the presence of a 2,2-dimethylchromen residue [3] in ring A. This was further supported by IR absorption at 1390 and 1375 cm⁻¹ for a gem-dimethyl group. The ¹H NMR spectrum also showed a singlet at δ 3.92, integrating for three protons, due to a methoxyl and a singlet at δ 6.64, due to an aromatic proton, which suggested a 5,7,8- or 5,6,7-substitution pattern for ring A. That candidin is 5methoxy-2",2"-dimethylpyrano(5",6": 7, 8)-flavone (1) was established by its partial synthesis from its corresponding flavanone, pongachin. Selenium dioxide dehydrogenation [4] of pongachin yielded a pure flavone which was identical with a natural sample of candidin in all respects (mp, mmp, co-TLC and co-IR).

1, Candidin

The isolation of candidin is of biogenetic interest because the corresponding chalcone and flavanone, pongachalcone-I and pongachin, have been isolated [1] from this source.

EXPERIMENTAL

Isolation. Air-dried, coarsely powdered seeds (1 kg) of T. candida were extracted with EtOAc after thorough treatment with petrol to remove most of the petrol soluble waxes. This extract was concd under red. pres. and subjected to column chromatography over Si gel. On elution with C_6H_6 -EtOAc (9:1) it gave a white, crystalline compound (70 mg, mp 193 6°), candidin (1). TLC: R_f 0.22 (C_6H_6 -EtOAc, 4:1), 0.45 (C_6H_6 -MeCOMe, 4:1), 0.64 (C_6H_6 -EtOAc, 1:1); UV $\lambda_{\max}^{\text{MeOH}}$ nm: 235, 270, 345; IR ν_{\max}^{RBr} cm⁻¹: 1630, 1590, 1395, 1380, 1335, 1110 and 770; ¹H NMR (90 MHz, CDCl₃): δ 1.50 (6 H, s, \gt C(Me)₂), 3.92 (3 H, s, OMe), 5.58 (1 H, d, J = 10 Hz, H-3"), 6.30 (1 H, s, H-3), 6.64 (1 H, s, Ar-H-6), 6.80 (1 H, d, J = 10 Hz, H-4"), 7.60 (5 H, s, B-ring protons).

Partial synthesis. Pongachin (50 mg), dry SeO₂ (75 mg) and dry amyl alcohol (7.5 ml) were refluxed for 12 hr. The mixture was then filtered and the residue passed through a column of Si gel. On elution with $\rm C_6H_6-EtOAc$ (9:1), crystals of candidin (mp 192–4°) were obtained, which had the same chromatographic and spectroscopic properties as the natural sample.

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