Phytochemistry, Vol. 25, No. 4, pp. 961–962, 1986.
Printed in Great Britain.

0031–9422/86 \$3.00 + 0.00

CANDIDONE, A FLAVANONE FROM *TEPHROSIA CANDIDA*

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(*Received* 10 *July* 1985)

Key Word Index—*Tephrosia candida*; Leguminosae; stems and leaves; candidone; ovalichalcone; dehydrorotenone.

Abstract—Candidone, ovalichalcone and dehydrorotenone have been isolated and identified from the stems and leaves of *Tephrosia candida*.

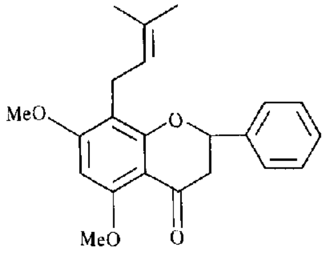
INTRODUCTION

The genus *Tephrosia* is reputed to possess pesticidal properties [1] and is also known to elaborate rotenoids and flavonoids [2]. From the roots, seeds and aerial parts of *T. candida*, several flavonoids have already been reported [3–9]. As a part of our programme on plants possessing pesticidal activity, we became interested to examine the stems and leaves of *T. candida**. In the present communication we report the isolation and structure elucidation of a new prenylated flavanone designated as candidone (**1**) along with ovalichalcone (**2**) [10], dehydrorotenone (**3**) [11] and β-sitosterol from the said parts of this plant. Interestingly, the occurrence of ovalichalcone (**2**) and dehydrorotenone (**3**) is being reported for the first time in *T. candida*.

RESULTS AND DISCUSSION

Candidone (**1**) crystallized from benzene–petrol as colourless needles, analysed for $C_{22}H_{24}O_4$ ($[M]^+$ m/z 352), mp 103°. The colour reaction (positive Shinoda test) and UV spectrum (λ_{max}^{EtOH} 240, 287 and 343 nm) together with the appearance of a double-doublet (H-2, δ5.38, J = 13.5 Hz) and a multiplet (C-3, 2H, δ2.90) in the 400 MHz NMR spectrum confirmed the presence of a flavanone system [12]. The appearance of a symmetrical multiplet at δ7.5 (5H) corresponded to an unsubstituted phenyl group. Functional group analysis revealed the presence of two methoxyl groups (δ3.90, 3.92, 6H) and a 1H-singlet at δ6.12 for the H-6. The remaining protons were observed as a doublet at δ1.67 (6H, J = 6 Hz) for a *gem*-dimethyl group, one doublet at δ3.28 (2H, J = 7 Hz) for methylene protons and a triplet at δ5.14 (1 H) for an isolated olefinic proton. These reasonances are typical of a prenyl side chain [13].

The mass spectrum showed two peaks at m/z 248 $[M - CH_2{=}CH{-}C_6H_5]^+$ and 205 $[M - CH_2{-}CH{=}CMe_2$



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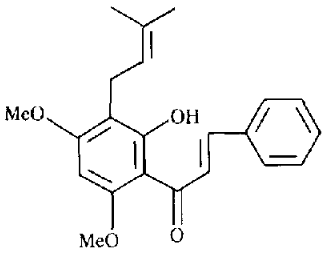

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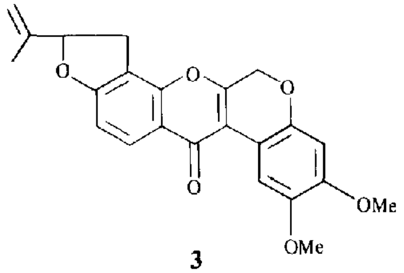

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*The plant material used in this investigation was obtained from the United Chemicals and Allied Products, 10, Clive Row, Calcutta-1, where a voucher specimen is preserved.

$-C_6H_5]^+$ corresponding to the loss of styrene and an isopentenyl group together with a phenyl fragment also confirmed that the B-ring of candidone (**1**) was unsubstituted. On the basis of these spectral evidence, candidone may be assigned as **1** or its 6-prenyl isomer.

The structure **1** was confirmed by converting it to ovalichalcone (**2**) by adsorbing **1** in a silica gel column for 24 hr. The column on elution with benzene–ethyl acetate (9:1) afforded a compound, the spectral data of which were found to be identical with ovalichalcone (**2**) in all respects. Thus, **1** is the corresponding flavanone of **2**.

EXPERIMENTAL

Dried stems and leaves (2.5 kg) were extracted with petrol (60–80°) and the concd extract chromatographed over silica gel. C_6H_6–EtOAc (9:1) eluates afforded first a pale yellow crystalline compound, mp 213–214° which was identified as dehydrorotenone by direct comparison with an authentic sample (co-TLC and superimposable IR). Further elution with the same solvent furnished a thick solid mass which on rechromatography over silica gel yielded ovalichalcone (**2**) and candidone (**1**), respectively.

Ovalichalcone (**2**). Mp 125–126°, crystallized from C_6H_6–petrol, analysed for $C_{22}H_{24}O_4$ ($[M]^+$ 352); UV λ_{max}^{EtOH} nm 331; $+AlCl_3+HCl$: 349. IR ν_{max}^{KBr} cm^{-1}: 1630 (α,β-unstd ketone). MS m/z: 352 $[M]^+$, 248 $[M-H_2C{=}CH{-}C_6H_5]^+$, 337 $[M-Me]^+$, 275 $[M-C_6H_5]^+$ 233 $[M-104-15]^+$. ^{1}H NMR (400 MHz, $CDCl_3$), δ 1.72 (*d*, 6H, J = 7 Hz $Me_2C{=}$), 3.89 (*s*, 3H, OMe), 3.94 (*s*, 3H, OMe), 3.29 (*d*, 2H, J = 2 Hz, $-CH_2-CH{=}C$), 5.13 (*m*, 1H, CH=C), 5.99 (*s*, 1H, H-5), 7.21–7.64 (*m*, 5H, 5 ArH), 7.8 (*d*, 2H, J = 1.7 Hz, *trans*-olefinic). Identity of **2** was confirmed by direct comparison with an authentic sample (co-TLC and superimposable IR).

Candidone (**1**). mp 103°, crystallized from C_6H_6–petrol, analysed for $C_{22}H_{24}O_4$: UV λ_{max}^{EtOH} nm: 343, 287, 240. IR ν_{max}^{KBr}: 1620 cm^{-1}. MS m/z: 352 $[M]^+$, 274 $[M-H-C_6H_5]^+$, 248 $[M-C_6H_5-CH{=}CH_2]^+$, 220 $[M-104-CO]^+$, 233 $[M-104-Me]^+$, 205 $[M-104-15-CO]^+$, 191 $[M-77-15-\text{isopentyl}]^+$. ^{1}H NMR (400 MHz, $CDCl_3$: δ 1.67 (*d*, 6H, J = 6 Hz, *gem*-dimethyl), 3.90 (*s*, 3H, OMe), 3.92 (*s*, 3H, OMe), 3.28 (*d*, 2H, J = 7 Hz, $-CH_2-CH{=}C$), 5.14 (*t*, 1H, J = 1 Hz, CH=C–) 7.5 (*m*, 5H, 5 ArH), 6.12 (*s*, 1H, H-6).

Acknowledgements—The authors are thankful to UGC, New Delhi, India for awarding fellowships to M.R. and S.R.M. They are also grateful to Professor M. Krishnamurti, Delhi University, for the gift of an authentic sample of ovalichalcone.

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