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FLAVONOID CONSTITUENTS OF *EUPATORIUM ODORATUM*

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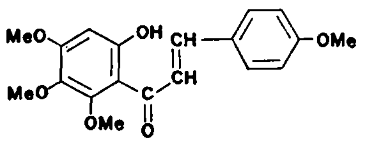
Abstract—Isosakuranetin and a new chalcone, odoratin, have been isolated from the leaves of *Eupatorium odoratum*. The structure of odoratin has been shown to be 2′-hydroxy-4,4′,5′,6′-tetramethoxy chalcone.

INTRODUCTION

The isolation of ceryl alcohol and β-sitosterol[1] and aromatic acids[2] from the leaves of *Eupatorium odoratum* (*Compositae*) was reported earlier. The present communication reports the isolation from the leaves of the same plant of a flavanone, isosakuranetin[3] and a new chalcone, called odoratin, whose structure has been shown to be (I). The flavonone, $C_{16}H_{14}O_5$ (M^+ 286), m.p. 179°, isolated from acetone extract by column chromatography over silica gel, formed a dimethyl ether, $C_{18}H_{18}O_5$, m.p. 120–121°. It was identified as isosakuranetin by comparison of m.m.p., TLC, UV and IR spectra with an authentic sample.

Odoratin (I), orange in colour, $C_{19}H_{20}O_6$, (M^+ 344), m.p. 142–144°, isolated from light petroleum (l.p. 60–80°) extract by column chromatography over silica gel, did not respond to Shinoda's test, but gave positive ferric chloride colour test. Its UV spectrum [λ_{max}^{EtOH} 360 (log ϵ 4·37), 305 (sh, log ϵ 4·01) and 237 nm (log ϵ 4·14)] was very characteristic of a chalcone. The bathochromic shift ($\lambda_{max}^{EtOH-AlCl_3}$ 378, 240 nm) of bands on addition of $AlCl_3$ indicated the presence of a free 2′-OH group in odoratin.



(I)

The NMR spectrum of odoratin (60 MHz in $CDCl_3$) showed two *trans*-olefinic protons (H-α and H-β) at 7·84δ as a singlet rather than the usual doublet (see NMR spectrum of 2′-hydroxy-4,4′,6′-trimethoxy chalcone[4]). One phenolic proton appeared as a singlet at 13·5 δ (disappeared on D_2O-exchange) which indicated that the –OH group is *ortho* to the

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[1] M. Ahmad and M. N. Nabi, *Sci. Res. Dacca, Pak.* **4** (2–3), 154 (1967).

[2] M. Ahmad and M. N. Nabi, *Sci. Res. Dacca, Pak.* **6** (1–2), 37 (1969).

[3] M. Hasegawa and T. Shirato, *J. Am. Chem. Soc.* 3557 (1955).

[4] T. J. Mabry, K. R. Markham and M. B. Thomas, *The Systematic Identification of Flavonoids*, p. 337, Springer, Berlin (1970).

carbonyl group. The signals at 3·82 (*s*, 3H), 3·85 (*S*, 3H) 3·93 (*s*, 3H) and 3·9 δ (*s*, 3H) were due to the protons of the four methoxyl groups. The H-2 and H-6 protons appeared at 7·59 δ (2H, *d*, *J* 9 Hz) and H-3 and H-5 protons appeared at 6·86 δ (2H, *d*, *J* 9 Hz). The H-3′ proton appeared as a singlet at 6·27 δ. Thus the NMR spectrum was in conformity with the structure (I) proposed for odoratin.

The MS of odoratin exhibited, besides the molecular ion peak at *m/e* 344, prominent peaks at 211, 210, 134 and 133 commensurate with the expected products from the proposed structure (I).

Seshadri *et al.*[5] reported the synthesis of 2′-hydroxy-4,4′,5′,6′-tetramethoxy chalcone, and the synthetic sample was found to be identical with odoratin in all respects (m.p., TLC, UV and IR spectra). This is the first report of the isolation of the above chalcone from a natural source.

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[5] N. NARASHIMHACHARI, V. D. NAGESWARA SASTRI and T. R. SESHADRI, *Proc. Ind. Acad. Sci.* 29A, 404 (1949).