Asian Journal of Chemistry Vol. 7, No. 4 (1995), 795–797

Two New Coumarins from *Setaria italica* Leaves and Study of Their Antimicrobial Activity

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Two new coumarins have been isolated from the leaves of *Setaria italica*. Their structures were elucidated as 6,7-dimethoxycoumarin and 5,8-dimethoxycoumarin on the basis of their spectral and chemical analysis. These coumarins were also subjected to their antimicrobial activities against various gram positive and gram negative bacteria.

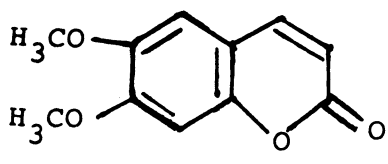
INTRODUCTION

Setaria italica Beauv (Graminae), which is commonly known as "Kauni" in Hindi, has wide distribution in India, China, Japan, South Africa, East Europe and North America[1]. The plant is considered to be a sweet, acrid and aphrodisiac drug and is used as a sedative to the gravid uterus[1]. Recently we have reported a new flavone glycoside, setaricin[2], and a new coumarin[3] from this plant. In the course of our investigations on the biologically active constituents of Indian traditional medicines, we have isolated two new coumarins from the leaves of *S. italica, i.e.*, 6,7-dimethoxy coumarin and 5,8-dimethoxy coumarin.

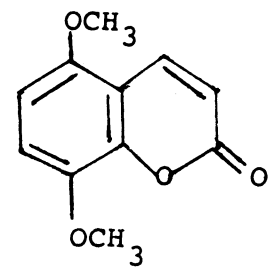
EXPERIMENTAL

Air dried and coarsely powdered leaves of *S. italica* (2.5 kg) were extracted with MeOH in a soxhlet. The concentrated methanolic extract was treated with $CHCl_3$, EtOAc and *n*-butanol. Each extract was worked up separately.

The concentrated $CHCl_3$ portion showed two spots on TLC examination over Si-gel (Benzene-EtOAc (1:1) as developing solvent) therefore it was chromatographed over silica-gel using benzene-ethylacetate gradient as eluant. Elution of the column with benzene-ethylacetate (7:3) yielded compound 1, which was crystallized from MeOH-ether as cream coloured powder (175 mg). The C_6H_6-



(1)



(2)

EtOAc (1:1) eluant gave compound 2, which was crystallized from $CHCl_3$-MeOH as white needles.

RESULTS AND DISCUSSION

Compound 1, m.p. 112–113°C, analysed for $C_{11}H_{10}O_4$ (Found: C, 64.10 H, 4.83, whereas $C_{11}H_{10}O_4$ requires C, 64.07, H, 4.85%); UV (MeOH) (nm) λ_{max}: 220, 265, 276, 303 and 338; IR (KBr) (cm^{-1}) ν_{max}: 2890, 1728, 1630, 1572, 1495, 1365, 1250, 1190, 995, 848; ^{1}H-NMR ($CDCl_3$, 270 MHz) δ: 7.420 (1H, s, H-5), 7.312 (1H, s, H-8), 7.52 (1H, d, J = 9.0 Hz, H-4), 6.50 (1H, d, J = 9.0 Hz, H-3), 3.97 (3H, s, OCH_3-7), 3.99 (3H, s, OCH_3-6); MS: M/z 206 $[M]^+$ ($C_{11}H_{10}O_4$), 178, 151, 152, 31.

Compound 2, analysed for $C_{11}H_{10}O_4$, m.p. 130–131°C (Found: C, 64.09; H, 4.81 whereas $C_{11}H_{10}O_4$ requires C, 64.07, H, 4.85%); UV (MeOH) (nm) λ_{max}: 250, 268, 279, 300 and 335; IR (KBr) (cm^{-1}) ν_{max} (cm^{-1}): 2890, 1728, 1630, 1570, 1195, 985, 840; ^{1}H-NMR ($CDCl_3$, 270 MHz) δ: 7.17 (1H, d, J = 8.5 Hz, H-6), 7.61 (1H, d, J = 8.5 Hz, H-7), 6.50 (1H, d, J = 9.0 Hz, H-3), 6.72 (1H, d, J = 9.0 Hz, H-4), 3.95 (6H, s, OCH_3–5 and OCH_3–8).

Both compounds 1 and 2 did not show positive test with $FeCl_3$ solution. Their IR spectrum exhibited bands characteristic of a coumarin; a band at 1728 cm^{-1} was assigned to an unsaturated lactone; peaks at 1630, 1572, 1495 cm^{-1} were due to aromatic C—C stretching of a coumarin skeleton[4]. Both coumarins 1 and 2 did not react with any acetylating and diazomethane indicating the absence of any free hydroxyl group in both compounds 1 and 2. Compounds 1 and 2 have similar molecular formula, UV and IR data, but differ only in their ^{1}H-NMR values. It means 1 and 2 have same groups but arranged differently. Presence of two methoxyl groups in both 1 and 2 was confirmed by IR (a peak at 2890 cm^{-1}) and ^{1}H-NMR (peaks at 3.99 and 3.97). Estimation of methoxyl groups when done by Zeisel's method[5] (21.15%) confirmed the presence of two methoxyl groups in compounds 1 and 2.

In the light of the above spectroscopic data, the structures of 1 and 2 were assigned as 6,7-dimethoxy coumarin (1) and 5,8-dimethoxy coumarin (2).

Antimicrobial activity

The compound 1 was screened for its antibacterial and antifungal activities using cup-plate method[6] at 100 μg concentration against the gram positive bacteria *Staphylococcus aureus*, *Staphylococcus citrus* and the gram negative bacteria *Escherichia coli*, *Salmonella typhosa* and fungi *Aspergillus niger* and *Neurospora cressa*. Under identical conditions the standard antibiotic chloromycetin showed a zone of inhibition of 30 to 35 mm, streptomycin 20 to 25 mm and penicilin-G 20 to 23 mm against the various strains of bacteria and fungi at 1000 μg concentration. Compound 2 showed moderate activity against different strains of bacteria and fungi (inhibition zone 15–23 mm).

ACKNOWLEDGEMENT

The authors are grateful to Prof. S.P. Banerjee, Head, Department of Chemistry for providing laboratory facilities.

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(*Received*: 21 December 1994; *Accepted*: 27 April 1995) AJC-957