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AN OPTICALLY ACTIVE CHROMANONE FROM *GYNURA FORMOSANA*

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Key Word Index—*Gynura formosana*; Compositae; aerial parts; chromanone.

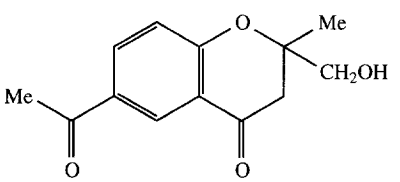
Abstract—A new optically active chromanone, isolated from the fresh aerial parts of *Gynura formosana*, has been characterized as 6-acetyl-2-hydroxymethyl-2′-methylchroman-4-one, by means of spectroscopic methods.

INTRODUCTION

Gynura formosana, a popular vegetable, is cultured throughout Taiwan and is used as a folk medicine. Phytochemical examination of this species has not yet been conducted, but the literature has reported a few interesting components, such as pyrrolizidine alkaloids, a terpene coumarin and several new spirost-5-ene derivatives from other *Gynura* species [1–3]. We describe the isolation and structure elucidation of a new chromanone (**1**) from the ethyl acetate extract of *G. formosana*.

RESULTS AND DISCUSSION

Compound **1**, mp 79–80°; molecular formula $C_{13}H_{14}O_4$ (HRMS: M^+ calc: 234.0892, found: 234.0884); [α] +11.45; the UV λ_{max} at 271, 312 (sh), 320 nm and IR ν_{max} at 1680 cm^{-1} (br.) depicted the 6-acetylchromanone skeleton of it [4], the ^1H NMR spectrum (in $CDCl_3$) exhibited one three proton singlet at δ 1.32 and another three proton singlet at 2.53, the latter indicating an acetyl methyl group attached to the benzene ring. One set of AB quartet signals at δ 3.59, 3.79 (each *d*, $J = 12$ Hz) corresponding to a CH_2OH group protons, which was confirmed by the appearance of a $[M - 31]^+$ peak at *m/z* 203 due to the loss of the CH_2OH group from the M^+ at *m/z* 234. The NOE spectrum showed the adjacent correlation of the high field methyl group (at 1.32) with the hydroxymethyl protons which indicated they were both substituted at the C-2 position. Another AB quartet at δ 2.53, 3.14 (each *d*, $J = 16$ Hz) was the C-3 non-equivalent two protons due to the asymmetric center generated at C-2 carbon. In the down-field region, three aromatic protons at δ 8.38 (*d*, $J = 2.5$ Hz), 8.08 (*dd*, $J = 9$ and 2.5 Hz), 6.96 (*d*, $J = 9$ Hz) indicated one 1,2,4-trisubstituted benzene ring. On the basis of the aromatic proton, especially the one at δ 8.38, it was concluded the acetyl group must be attached to the benzene ring at C-6. The structure of **1** is established as 6-acetyl-2-hydroxymethyl-2′-methylchroman-4-one. The absolute configuration has not been determined.



1

EXPERIMENT

Isolation. The aerial parts of *G. formosana* Kitamura were collected in Hsing-Chu, Taiwan. A voucher specimen (TCB68516) was deposited in the Herbarium of the Department of Botany, National Chung-Hsing University. The air-dried material was extracted with hot methanol. After concentration, the crude extract (15 g) was dissolved in *n*-hexane, the insoluble residues were re-dissolved in EtOAc. The EtOAc extracts were successively chromatographed over silica gel to obtain a light yellow solid **1** (R_f: 0.13, hexane–EtOAc, 7:3) (8 mg).

6-Acetyl-2-hydroxymethyl-2′-methylchroman-4-one (**1**). Mp 79–80°C; [α] +11.45 (*c* 0.039); UV λ_{max} (log ε): 240 (4.0), 271 (3.7), 312 (sh), 320 (3.0) nm; IR ν_{max}: 3428, 2928, 2860, 1682, 1608, 1254 cm^{-1}; MS *m/z* (%): 234 $[M]^+$ (41), 219 (4), 203 $[M - 31]^+$ (100), 163 (38), 147 (20); ^1H NMR (300 Mz, $CDCl_3$): 1.32 (*s*, 3H, -Me), 2.53 (*s*, 3H, CO-Me), 2.53 (*d*, 1H, $J = 16$ Hz, H-3a), 3.14 (*d*, 1H, $J = 16$ Hz, H-3b), 3.59

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(*d*, 1H, $J = 12$ Hz), 3.79 (*d*, 1H, $J = 12$ Hz), 6.96 (*d*, 1H, $J = 9$ Hz, H-8), 8.08 (*dd*, 1H, $J = 9$ Hz and 2.5 Hz, H-7), 8.38 (*d*, 1H, H = 2.5 Hz, H-5); ^{13}C NMR: 20.4 (*q*), 26.3 (*q*), 43.5 (*t*), 68.4 (*t*), 82.8 (*s*), 118.9 (*d*), 119.3 (*s*), 128.1 (*d*), 130.7 (*s*), 135.6 (*d*), 163.0 (*s*), 191.5 (2), 196.3 (*s*).

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