Structure of Conyzorigun, a New Chromone from *Ageratum conyzoides*

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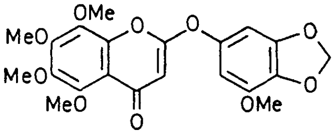
Summary The structure of a new highly oxygenated chromone conyzorigun has been determined, and shown to possess a novel keten acetal system.

PREVIOUS work on *Ageratum conyzoides* (Compositae) led to the isolation of β-sitosterol, stigmasterol, and friedelin,[1] and ageratochrome, 7-methoxy-2,2-dimethylchromen, and ageratochromen.[2] From the light petroleum extract of the stem and leaves of this shrub, we have isolated β-sitosterol, stigmasterol, tritriacontene ($C_{32}H_{64}$), 7-methoxy-2,2-dimethylchromen, and conyzorigun.

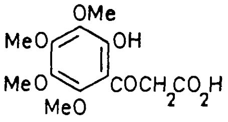
Conyzorigun, $C_{21}H_{20}O_{10}$, m.p. 192—193 °C, (needles from MeOH), ν_{max} 1638 cm^{-1}; λ_{max} 272 (ϵ 19,000) and 338 nm (ϵ 22,000), unaffected by base, a minor constituent of the plant (*ca.* 0·005%) was eluted from alumina with ether. The 60 MHz ^{1}H n.m.r. spectrum shows absorptions for OCH_2O (2H, s) at δ 6·02, vinyl H (1H, s) at δ 6·50; aromatic protons (2H, d, *J* 1 Hz) centred at δ 6·95 and 7·08 and 5 aromatic OMe groups (3H, s at δ 4·13, 4·03 and 4·00, and 6H, s at δ 3·99). ^{13}C N.m.r. absorptions at δ 56·8, 61·5, 61·7, 61·9, and 62·1 p.p.m. as well as the absence of low-field signals other than that at δ 176·9 attributed to a carbonyl carbon were taken as additional evidence for 5 aromatic OMe.

All the data can be accommodated by structure (**1**) and at least three isomeric structures. After conyzorigun had been refluxed for 6 h in 4M-NaOH in n-propanol and acidified, two products (A) and (B) were isolated in yields of 90 and 86% respectively. (A) was characterised as 2,3,4,5-tetramethoxy-6-hydroxyacetophenone from its ^{1}H n.m.r. spectrum [δ 2·67 (3H, s, COMe), 3·80, 3·85, 3·95, and 4·07 (each 3H, s, aromatic-OMe), and 13·13 (1H, s, exchangeable with D_2O, OH)]. (B) was similarly characterised as 3,4-methylenedioxy-5-methoxyphenol [acetate, M^+ *m/e* 210; ^{1}H n.m.r. δ 3·93 (3H, s, aromatic OMe), 6·05 (2H, s, OCH_2O), and 7·20 and 7·32 (2H, *J* 1 Hz, ArH)]. The structures assigned to (A) and (B) were confirmed by synthesis using appropriate modifications of synthetic methods used for identical or similar compounds.[3]

Compound (A) is thought to have arisen as a result of decarboxylation of the β-keto-acid (**2**) which together with (B) formed the initial hydrolysis products. Conyzorigun must therefore have structure (**1**).



(1)



(2)

To our knowledge such a highly oxygenated aromatic compound with a reasonably stable keten acetal system is without precedent in extractives from plants. However we feel conyzorigun is biogenetically related to the chromens which are abundant in the plant.

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