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Organic Chemistry

8-HYDROXY QUERCETAGETIN FROM PETALS OF TAGETES ERECTA

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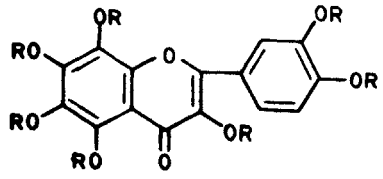
A new polyhydroxy compound isolated from the ethanolic extract of the petals of *T. erecta* was constituted as 3,5,6,7,8 3′,4′-heptahydroxyflavone (8-hydroxy quercetagetin) (I) on the basis of its colour reactions and spectral data.

Keywords : 8-Hydroxy Quercetagin; Tagetes Erecta; IR Spectrum; UV Spectrum

INTRODUCTION

Tagetes erecta (Compositae) had been examined earlier by a group of workers (Mahal, 1938; Morita, 1957; Pankajamani *et al.*, 1953; Perkin, 1913*a*, *b*; and Rao *et al.*, 1941). The present communication now reports the isolation and characterisation of a new flavonol derivative (1) from its petals. **1** crystallised from ethanol as yellow needles, m.p. > 330°. Colour reactions and UV spectral data showed it to be a flavonol derivative. Strong absorbtion bands in the IR spectrum of **1** at 3448 and 1653 cm^{-1} indicated the presence of hydroxyl(s) and flavonoid carbonyl function(s) respectively. The shifts observed in the UV spectrum of **1** in methanol (λ_{max}: 255, 370nm) on additions of NaOAc, $AlCl_3$, $AlCl_3$—HCl, NaOMe as well as NaOAc—H_3BO_3 in the separate recordings, indicated the presence of hydroxyls at C–7 C–3 and/or C_5 and C–4 positions along with an ortho–dihydroxyl grouping. Positive Gossypetone (Perkin, 1913) as well as Quastel (Quastel, 1931) tests supported the presence of a para–as well as an orthodihydroxy grouping respectively in **1**. Positive Bargellini test (Bargellini, 1919) indicated a vicinal trihydroxy grouping.

The acetate (**Ia**) of **1** crystallised from chloroform-petroleum ether as colourless needles, m.p. 160°; analysed for $C_{29}H_{24}O_{16}$. Pmr spectrum of **Ia** showed seven phenolic acetoxyl functions (δ 2.1–2.5) and three aromatic protons. The signal at δ 7.3 for one proton was attributed to C–5′ proton whereas the signal at δ 7.45 integrating for two protons was characterised due to the protons at C–2′ and C–6′ positions. Since the three aromatic protons were located at C–2′, C–5′ and C–6′



I, R = H
Ia, R = $COCH_3$

positions, the seven acetoxyls were considered to be present at the remaining C-3, C-5, C-6, C-7, C-8, C-3′ and C-4′ positions. Consequently, **1** was assigned its structure as 3,5,6,7,8,3′, 4′-heptahydroxyflavone (**1**). The co-occurrence of **1** with luteolin, patuletin, quercetin and quercetagetrin in *T. erecta* is of great biogenetic interest. The occurrence of heptahydroxyflavone (I) in this plant material may be considered to arise by the nuclear hydroxylation of 3,5,6,7,3′,4′-hexahydroxyflavone (Quercetagetin).

Experimental

Air-dried petals of *T. erecta* were extracted first with pet. ether to remove wax and colouring matters, and then with ethanol. The solvent-free ethanolic extract was further treated with pet. ether to remove the last traces of colouring matters and finally with ether and ethyl acetate in succession. The combined ether and ethyl acetate soluble fraction yielded three major known phenolic components, luteolin, patuletin and quercetagetin alongwith **1**. The residue of the ethanolic extract left behind after extraction with ethyl acetate yielded quercetagetrin. The four non-glycosidic components were separated by the preparative thin layer chromatography as their acetates using silica-gel as an adsorbent and benzene : methanol (45 : 5) as the solvent system. The four acetates thus obtained were deacetylated with methanol-hydrochloric acid (5 per cent) to obtain the corresponding hydroxy compounds.

1 crystallised from ethanol as yellow needles, m.p. > 330° (Found : C, 54.2; H, 3.4. $C_{14}H_{10}O_9$ requires C, 53.90; H, 3.02 per cent). IR (KBr) : 3448, 2857, 1724, 1653, 1550, 1493, 1290, 1176, 1078, 1058, 1036, 995, 971, 943,917, 877, 855, 813, 787, 755, 730 cm^{-1}. UV (MeOH) : 255, 370nm; $+AlCl_3$: 270, 400nm; $+ AlCl_3 +$ HCl : 265, 390nm; +NaOAc : 245, 275(sh), 385nm: + NaOAc + H_3BO_3 : 260, 390nm; + NaOMe : 285, 400(d)nm.

1a (acetate of **1**) crystallised from chloroform-petroleum ether as colourless needles, m.p. 160° (Found : C, 55.4; H, 4.0. $C_{29}H_{24}O_{16}$ requires C, 55.41; H, 3.81 per cent). Pmr (δ, $CDCl_3$, at 60 MHz): 2.1 (3H, s, $-OCOCH_3$), 2.44 (15H, *bs* 5 X $-OCOCH_3$), 2.5 (3H, s, $-OCOCH_3$), 7.3 (1H, *d*, J = 9 Hz, $C_{5'}$-H), 7.45 (2H, *m*, $C_{2'}-H$, $C_{6'}-H$).

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