Short Communication

A New Flavone from the Leaves of Rohida (Tecomella undulata)

M. Mohibbe Azam and Abu Ghanim
Central Arid Zone Research Institute, Jodhpur 342 003, India.

*Tecomella undulata* (Smith) Seeman (syn. *Tecoma undulata* G. Don, Bignoniaceae), locally known as Rohida, is one of the co-dominant species in the desert of western Rajasthan and Haryana. The plant parts are used in a variety of ailments (Anonymous, 1976). Previous investigations (Verma et al., 1986; Azam, 1999; Azam and Ghanim, 2000) have revealed the presence of lapachol, dehydrotechtol, triacontanol, n-hentriacontanol, betulinic acid, oleanolic acid, ursolic acid, cirsimaritin, cirsilineol, β-sitosterol, quinones, chromone glucoside, etc., in different parts of *T. undulata*. Present work describes the isolation and structure elucidation of a new flavone, 5, 4′-dihydroxy-6, 8, 3′-trimethoxyflavone (compound-I), from leaves of the plant.

Melting points were uncorrected. EIMS were obtained on a Varian Mat 331A mass spectrometer at 70 EV. $^1$H NMR spectra were recorded on Jeol JNM Fx-200 FTNMR spectrometer. Chemical shifts were recorded in δ (ppm) with TMS as an int. standard. UV and IR were recorded on Carl Zeiss specord UV-VIS and 75 IR spectrophotometer, respectively. The leaves of *T. undulata* were collected from CR Farm of the Institute.

Air-dried leaves (4.4 kg) were powdered and extracted in a soxhlet apparatus with hot petrol (60-80°C). The residue after removal of solvent was chromatographed over a column of Silica gel and eluted with petrol (60-80°C) and petrol-EtOAc mixture of increasing polarity. Cirsimaritin, cirsilineol and the compound-I were obtained from fractions of petrol-EtOAc (3:1). Cirsimaritin, cirsilineol and the compound-I were separated by silica gel prep. TLC (1 mm thickness) using CHCl₃:MeOH (9:1). Physical properties and spectral data of 5, 4′-Dihydroxy-6, 8, 3′-trimethoxyflavone (compound-I) are as follows: - Crystallized from MeOH as reddish yellow crystalline solid (30 mg), m.p. 180°C. $\lambda_{max}$ (nm) (MeOH): 255 sh, 279, 346.3; +AlCl₃: 260, 286.7, 370.0; +AlCl₃/HCl: 257, 286, 366.5; + NaOMe: 271.7, 408.5; + NaOAc: 272.9, 369.2, 416.7; NaOAc/H₃BO₃: 277.8, 347.2. IR $\nu_{max}$ (CHCl₃) cm⁻¹: 3150, 1640, 1580. $^1$H NMR (200 MHz, DMSO-d₆) δ = 3.66 (s, 3H, 1x -OCH₃), 3.74 (s, 3H, 1x -OCH₃), 3.89 (s, 3H, 1x -OCH₃), 6.54 (s, 1H, H-7), 6.60 (s, 1H, H-3), 6.87 (d, J= 8.5 Hz, 1H, H-5′), 7.49 (m, 2H, H-2′ and H-6′), 10.15 (4′- OH), 12.30 (5-OH). EIMS m/e (%): 344 (M)$^+$ (85.07), 343(M-1)$^+$ (7.91), 329 (M-CH₃)$^+$ (100), 315(M-29)$^+$ (10), 301(M-43)$^+$ (1.5), 181(A₁-CH₃)$^+$ (11.9), 153(A₁-COCH₃)$^+$ (35).
Interpretation of UV, \(^1\)H NMR and MS spectra of compound-1 revealed that it is a dihydroxytrimethoxyflavone (C\(_{18}\)H\(_{16}\)O\(_7\)) with molecular ion at m/e 344. Hydroxyl groups at C-5 and C-4' were indicated in UV spectrum with diagnostic reagents and confirmed by \(^1\)H NMR signals (12.30 ppm for 5-H and 10.15 ppm for 4'-H) (Mabry et al., 1970). A 3', 4'-dioxygenation pattern in B-ring of the flavone was indicated by two peaks in band II of UV spectra (255 sh, 279). It was confirmed by both alkaline decomposition and oxidation with H\(_2\)O\(_2\) that afforded vanillic acid. Thus, B-ring has 3'-OMe and 4'-OH substitutions. The observed bathochromic shift in UV spectra of compound-1 after addition of AlCl\(_3\)/HCl to its methanolic solution indicated the presence of a methoxyl group at C-6 with hydroxyl group at C-5 (Parmar et al., 1987). The high intensity of (M-CH\(_3\))^+ ion at m/e 329 (100%) supported the presence of methoxyl group at C-6 (Parmar et al., 1987). The presence of two singlets (6.54, s, 1H; 6.60, s, 1H) in \(^1\)H NMR spectra and MS fragments at m/e 181 and 153 showed that third methoxyl group is in A-ring. Thus A-ring is trisubstituted. From the discussion it follows that the compound-1 is either 5, 4'-dihydroxy-6, 8, 3'-trimethoxyflavone or 5, 4'-dihydroxy-6, 7, 3'-trimethoxyflavone. 5, 4'-Dihydroxy-6, 7, 3'-trimethoxyflavone is a known compound (cirsilineol/anisomelin) with m.p. 199-200°C (Devi et al., 1979) while the compound-1 has m.p. 180°C. Cirsilineol has also been isolated from the leaves of the plant (Azam and Ghanim, 2000). Thus, the compound-1 is 5, 4'-dihydroxy-6, 8, 3'-trimethoxyflavone. The structure was supported by negative reaction of the compound with Gibbs' reagent (King et al., 1957) and higher intensity (100%) of (M-CH\(_3\))^+ ion at m/e 329 in the MS (Parmar et al., 1987). To the best of our knowledge compound-1 is a new compound as it has neither been synthesized nor isolated from any natural source.

References


