Desmosdumotin B: A New Special Flavone from Desmos dumosus

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Abstract: A new special flavone, named desmosdumotin B, was isolated from the roots of *D. dumosus* and its chemical structure identified as 5-hydroxy-7-one-6,8,8-trimethylflavone by spectral analysis and X-ray.

Keywords: Annonaceae, Desmos dumosus, desmosdumotin B.

Desmos dumosus (Roxb.) Saff. is a liana-like or straight up shrub of the southern and the southwestern areas of China. The roots and leaves of *D. dumosus* are used as antimalarial, insect-killing, antirheumatic, antispasmodic and pain-relieving agent in Chinese folk medicine. Several flavonoids have been isolated from the plant¹⁻⁶. In this paper we report the isolation and structural elucidation of a new compound, 5-hydroxy-7-one-6,8,8-trimethyl flavone, named desmosdumotin B.

Desmosdumotin B, yellow crystal, mp: 217-218°C. It was assigned to have a molecular formula of C₁₈H₁₆O₄ by EI-MS (M⁺ m/z 296) and elemental analysis (which showed C, 72.91; H, 5.50. calcd. for C, 72.96; H, 5.44). UV spectrum λ max (MeOH) nm: 215, 287. The IR spectrum revealed the presence of conjugated carbonyl group (1700, 1650cm-1), aromatic rings (1620,1460cm-1). ¹H NMR spectrum showed the presence of a chelated hydroxy group (δ 13.10, s,); an aromatic methyl group (δ 1.87, s,); unsubstituted aromatic ring (δ 7.54-7.84, m,); one olefinic proton (δ 6.91, s,) and two equal methyl groups (δ 1.59, s,). In ¹³C NMR spectrum 18 carbon signals were observed including nine quaternary carbon, six methine and three methyl. HMQC showed that the signal at δ 6.9 ppm belongs to aromatic methyl, 25.2 ppm belongs to two equal methyl groups, 110.1 ppm belongs to C-3 chemical shift. HMBC showed proton of hydroxy correlated with C-5, C-10 and C-6 (δ 163.5, 110.4 and 108.4ppm); proton of aromatic methyl correlated with C-7, C-5 and C-6 (δ 196.1, 163.5 and 108.4ppm); protons of two equal methyl correlated with C-7, C-9 and C-8 (§ 196.1, 174.0 and 47.2ppm); proton at 6.91ppm(H-3) correlated with C-1', C-2 and C-4(δ 132.5, 164.3 and 180.7ppm). ¹³C NMR (CDCl₃, TMS) δ ppm: 6.9 (C-6-CH₃), 25.2 (C-8-2CH₃), 47.2 (C-8), 108.4 (C-6), 110.1 (C-3), 110.4 (C-10), 125.9 (C-2', C-6'), 129.4 (C-3', C-5'), 129.9 (C-4'), 132.5 (C-1'), 163.5 (C-5), 164.3 (C-2), 174.0 (C-9), 180.7 (C-4), 196.1 (C-7). EI-MS m/z (%): 296 (M⁺, 100), 281 (M⁺-CH₃, 91), 268 (M⁺-CO, 48), 253

 $(M^+\text{-CO-CH}_3, 96)$, 240 $(M^+\text{-CO-CO}, 21)$, 105 (9), 77 (2). From the above results, the new compound was determined to be 5-hydroxy-7-one-6,8,8 -trimethylflavone, named desmosdumotin B. The result of X-ray single crystal diffraction of this compound is completely in agreement with the spectral analysis.

Figure 1

References

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