6-Oxygenated flavones from *Baccharis trinervis* (Asteraceae)

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1. Subject and source

*Baccharis trinervis* (Lam.) Pers. (Family: Asteraceae alt. Compositae), used in South American folk medicine as an antiseptic, digestive and to treat snake-bites (Duke, 1999), is widely distributed from Mexico to Argentina (USDA-ARS-GRIN database, 1999). Plant material was collected from Costa Rica and supplied by Biotics Limited, University of Sussex, Brighton, UK. A voucher specimen (MNL10118) has been maintained at the herbarium of the Institute of Grassland and Environmental Research (IGER), Aberystwyth, UK.

2. Previous work

Previous phytochemical studies on *B. trinervis* established the presence of flavones (Herrera et al., 1996; Arriaga-Giner et al., 1982) and neoclerodane type diterpenes...
(Kuroyanagi et al., 1993; Jakupovic et al., 1986). Antiviral activity (Abad et al., 1999), anti-inflammatory and antioxidant properties (de las Heras et al., 1998) of this plant have also been reported.

3. Present study

The CH$_2$Cl$_2$ extract of branches of B. trinervis (0.78 kg) was fractionated by Biotage$^\text{TM}$ 75 flash chromatography on silica gel using a step gradient of increasing polarity: $n$-hexane–EtOAc–MeOH with nine fractions of 1000 ml. Reversed phase preparative HPLC (C$_{18}$ preparative column, eluted with a gradient — water : acetonitrile : 0.1% TFA in acetonitrile = 60 : 30 : 10–0 : 90 : 10 in 25 min, 55 ml/min, detection at 210 nm) of the flash fraction 5 (40% EtOAc in $n$-hexane) has yielded 5,7-dihydroxy-6,4'-dimethoxyflavone, (pectolinarigenin, 1, 6.8 mg) (Hase et al., 1995), 5-Hydroxy-6,7,4'-trimethoxyflavone (salvigenin, 2, 35.0 mg) (Hertz and Gibaja, 1972; Talpatra et al., 1974; Xaasan et al., 1980) and 5,4'-dihydroxy-3,6,7-trimethoxyflavone (penduletin, 3, 1.1 mg) (Wang et al., 1989). Compounds 1 and 3 were further purified by reversed phase semi-preparative HPLC (C$_{18}$ semi-preparative column, eluted isocratically with the solvent mixture water: 0.1% TFA in MeOH = 30 : 70, 25 mL/min., detection at 210 nm). Structures of all these compounds have been determined on the basis of UV, $^1$H NMR, $^{13}$C NMR, HMBC, HMQC and LC-MS data, and direct comparison with the respective literature data. Unambiguous assignment of $^{13}$C NMR data for salvigenin (2) has been presented for the first time.

Salvigenin (2). $^{13}$C NMR (125 MHz, CDCl$_3$): $\delta$ 182.9 (C-4), 164.2 (C-2), 162.9 (C-4'), 159.0 (C-7), 153.4 (C-9), 153.3 (C-5), 133.0 (C-6), 128.2 (C-2', C-4'), 123.8 (C-1'), 114.7 (C-3', C-5'), 106.4 (C-10), 104.3 (C-3), 90.8 (C-8), 61.0 (6-OMe), 56.5 (7-OMe), 55.7 (4'-OMe).

4. Chemotaxonomic significance

The genus Baccharis is well-known for producing flavones (Kuroyanagi et al., 1985; Kupchan and Bauerschmidt, 1971; Dictionary of Natural Products, 1999). While
several other flavones have been reported from *B. trinervis* (Herrera et al., 1996; Arriaga-Giner et al., 1982), none of the compounds (1–3) has previously been isolated from this species. However, compounds 1–3 have been reported from other genera within the Asteraceae (alt. Compositae) and also from other plant families (Dictionary of Natural Products, 1999). As flavonoids are an important class of compounds for plant systematic and evolutionary studies, the chemotaxonomic importance of the flavonoids (1–3) reported here deserves consideration.

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**References**


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