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A new lactone from *Senecio scandens*

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1. Subject and sources

Senecio plants (Compositae) are extensively used in single or formulated forms in Chinese traditional and folk medicine for antiinflammation, antibiosis, etc. There are about 100 species widely distributed in China with different morphological characteristics (Chen, 1999).

Senecio scandens Buch.-Ham. ex D. Don, locally known as ‘‘Qianliguang’’, is one of the most popular species used as a Chinese medicinal herb but the chemical components of this species have not been fully disclosed to date. The aerial parts of this plant were collected from Rongan county, Guangxi province of PR China in April 2005 and the vouchers have been deposited in the Herbarium of the Institute of Chinese Materia Medica, Shanghai University of Traditional Chinese Medicine.

2. Previous work

Pyrrolizidine alkaloids and sesquiterpenes with a furanoeremophilane skeleton have been reported as the major components from the genus of *Senecio* (Bohlmann et al., 1977). Pyrrolizidine alkaloids (Batra and Rajagopalan, 1977), phenolic acids (Wang and Tu, 1980) and jacaranone glycosides (Tian et al., 2006) have been previously isolated from *S. scandens*.

3. Present study

In the present study of *S. scandens*, a new lactone, (*E*)-seneciolactone (**1**), together with nine known compounds (**2**–**10**) were isolated and their structures determined based on spectral methods. The stereochemistry structures of seneciolactone (**1**) and (*E*)-cannabifolactone A (**2**) were firstly elucidated based on NOESY experiment.

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The air-dried aerial parts of *S. scandens* (6.0 kg) were exhaustively extracted with 80% ethanol under reflux. The extract was evaporated in vacuum to yield a syrupy residue (200 g). The residue was suspended in water (3000 mL) and partitioned with petroleum ether (3000 mL × 3), EtOAc (3000 mL × 5) and *n*-BuOH (3000 mL × 3) successively, to give the corresponding fractions (200 g, 300 g and 200 g), respectively.

A portion (270 g) of the EtOAc extract was subjected to column chromatography on silica gel (200–300 mesh, 2 kg) using stepwise elution with $CHCl_3$–MeOH (100:0, 50:1, 20:1, 10:1, and 1:1) to yield five fractions: Fr.1 (35 g) Fr.2 (40 g), Fr.3 (53 g), Fr.4 (41 g) and Fr.5 (78 g).

Fr.1 was chromatographed on silica gel (200–300 mesh, 1000 g) with a petrol ether–EtOAc gradient system (10:1–2:1) to give five sub-fractions (sub Frs.1A–1E). Sub Fr.1A was subjected to repeated column chromatography on silica gel by gradient elution with petroleum ether–EtOAc (5:1, 4:1, 3:1, 2:1) and purified by Sephadex LH-20 ($CHCl_3$–MeOH (1:1)) to afford compound **1** (8 mg), (*E*)-cannabifolactone A (**2**, 10 mg) (Wu et al., 2002), 4-methoxyphenylacetic acid (**3**, 10 mg) (Sadtler Research Laboratories Inc., 1969) and 2,5-dihydroxybenzeneacetic acid (**4**, 50 mg) (Yamaguchi et al., 1989), respectively. Sub Fr.1B (5 g) was subjected to repeated silica gel column chromatography (200–300 mesh) with a gradient of petroleum ether–EtOAc, followed by Sephadex LH-20 eluted with MeOH to yield jacaranone (**5**, 40 mg) (Bohlmann and Suwita, 1976), ethyl 2-(1-hydroxy-4-oxocyclohexa-2,5-dienyl) acetate (**6**, 40 mg) (Bohlmann and Suwita, 1976), methyl 2-(1-hydroxy-4-oxocyclohexyl) acetate (**7**, 70 mg) (Bohlmann et al., 1981) and ethyl 2-(1-hydroxy-4-oxocyclohexyl) acetate (**8**, 20 mg) (Bohlmann et al., 1981).

Fr.2 (20 g) was also subjected to repeated column chromatography on silica gel by gradient elution with petroleum ether–EtOAc (3:1, 1:1, 1:2, 0:1) to give 5-methoxybenzofuran-2(3*H*)-one (**9**, 27 mg) (Zbiral et al., 1965) and methyl 2-(1,4-dihydroxycyclohexyl)-acetate (**10**, 5.3 mg) (Wu et al., 2005).

The structures of the known compounds (**3**–**10**) were elucidated by comparison of their UV, ESIMS/EIMS, ^{1}H NMR, ^{13}C NMR, HMBC and HMQC data with the published data.

Compound **1** was obtained as a yellow powder. Mp. 80.4–82.5 °C; UV λ_{max} (MeOH): 197 nm, 362 nm; IR: 3420 cm^{-1} (ν_{OH}), 1767 cm^{-1} ($\nu_{c=o}$), 1718 cm^{-1} ($\nu_{c=o}$), 1610 cm^{-1}, 1629 cm^{-1}, 1470 cm^{-1} ($\nu\phi$).The molecular formula of **1** was assigned as $C_{16}H_{12}O_6$, from HREIMS spectrometry (*m*/*z* 300.0637, calcd 300.0634). The absorptions at 1767 cm^{-1} in the IR spectrum indicated the presence of a lactone structure. In the ^{13}C NMR spectrum, 16 carbon signals were observed as one methyl, one methylene, six methines and eight quaternaries. From ^{1}H NMR spectrum, we observed a typical ABX coupling system for a 1,2,4-trisubstituted aromatic ring [δ7.08 (1H, d, $J = 8.6$ Hz), 6.85 (1H, dd, $J = 8.6$, 2.4 Hz), 7.84 (1H, d, $J = 2.4$ Hz)], an α,α'-disubstituted furan ring substituted at positions of [7.35 (1H, d, $J = 3.5$ Hz), 6.85 (1H, d, $J = 3.5$ Hz)] and a methyl group [δ2.25 (3H, s)], respectively. The form of compound **1** was determined on the basis of a NOESY experiment, correlation between H-10 and H-12 was strong, but no correlation between H-10 and H-4 was observed, which indicated that the form was *E* type but not *Z* type, so the absolute structure of compound **1** was established as (*E*)-5-Hydroxy-3-[(5-acetoxymethyl-2-furanyl) methylene]-2(3*H*)-benzofuranone (Fig. 1; Table 1).

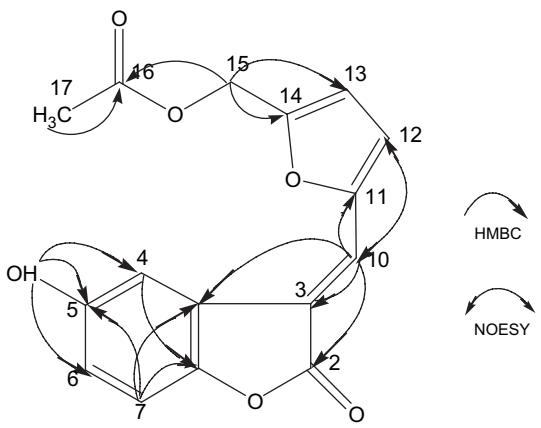

Fig. 1. Key HMBC and NOESY correlations for compound **1**.