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A new lactone from *Senecio cannabinifolius* less

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Note

A NEW LACTONE FROM *SENECIO CANNABIFOLIUS* LESS.

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A new lactone compound named cannabifolactone A was isolated from the water extract of the aerial parts of *Senecio cannabifolius* Less. Its structure was elucidated mainly by 1D- and 2D-NMR techniques.

Keywords: *Senecio cannabifolius* less; Compositae; Cannabifolactone A; Spectral data

INTRODUCTION

Senecio cannabifolius Less. (Compositae) is a perennial plant distributed in the Northeast of China, which contains large quantities of sesquiterpenoids and pyrrolizidine alkaloids [1]. Pharmacological researches have demonstrated the phenolic acid components have antimicrobial activities [2]. In this paper, we deal with the isolation and identification of a new lactone derivative, named cannabifolactone A (Fig. 1) from the water extract of the aerial parts of *S. cannabifolius* Less.

RESULTS AND DISCUSSION

Cannabifolactone A was obtained as a yellow powder. The EI-MS clearly revealed its molecular weight of 258 (100%, relative intensity) which had a formula of C₁₄H₁₀O₅ (HRMS: 258.0457, calcd; 258.0455, measured). The IR spectrum showed strong absorptions at 3227 cm⁻¹ (OH), 1758 cm⁻¹ (C = O), 1610, 1572, 1460 cm⁻¹ (aromatic ring). The ¹³C-NMR spectrum exhibited 14 resolved signals, comprising 1 × CH₂, 6 × CH and 7 × quaternary carbons, as distinguished by DEPT spectrum. Ten proton signals were present in the ¹H-NMR spectrum and two proton signals at δ 9.48 (1H, s) and δ 5.58 (1H, t, J = 5.8 Hz) disappeared in the D₂O exchange experiment, indicating that the compound

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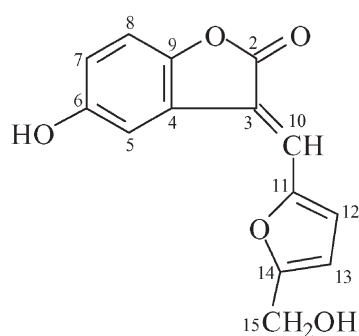


FIGURE 1 The structure of cannabifolactone A.

contains two exchangeable protons. With its IR spectrum, these two exchangeable protons may be assigned to two hydroxyl groups. The signals in the $^1\text{H-NMR}$ spectrum also showed a classical ABX coupling system for a 1,2,4-trisubstituted aromatic ring [δ 7.07 (1H, d, $J = 8.6\text{ Hz}$), 6.81 (1H, dd, $J = 8.6, 2.4\text{ Hz}$), 7.84 (1H, d, $J = 2.4\text{ Hz}$)], a furan ring is substituted at positions α, α' [δ 7.37 (1H, d, $J = 3.4\text{ Hz}$), 6.70 (1H, d, $J = 3.4\text{ Hz}$)] and a hydroxymethyl group [δ 5.58 (1H, t, $J = 5.8\text{ Hz}$), 4.70 (2H, d, $J = 5.8\text{ Hz}$)], respectively. Taking the HMQC and HMBC correlation spectra into account, we can establish the molecular structure of cannabifolactone A as Fig. 1.

EXPERIMENTAL

General Experimental Procedures

MP was obtained from a Yanaco micro-melting point apparatus (uncorrected). The IR spectral data were measured on a Bruker IFS-55 instrument (KBr). EI-MS was carried out with a JEOL-DX 302 mass spectrometer. 1D- and 2D-NMR spectra were recorded on a Bruker ARX-300 instrument with TMS as an internal standard.

Plant Material

The aerial parts of *S. cannabifolius* Less. were offered by Changchun Huakang Pharmaceutical Company Ltd. and identified by Prof. Z. K. Yan (The Research Institute of Changchun Traditional Chinese Medicine).

Extraction and Isolation

Air-dried aerial parts (30 kg) were powdered and extracted three times with H_2O . The extract was concentrated and partitioned between H_2O and CHCl_3 . The CHCl_3 portion (57 g) was fractionated by silica gel (200–300 mesh) chromatography eluted with CHCl_3 –MeOH (from 100:0 to 1:1) to afford several fractions. The fraction from CHCl_3 –MeOH (100:1) gave 23 mg of cannabifolactone A as a yellow powder.

Identification

Cannabifolactone A: yellow powder, mp 224–226°C (acetone); EI-MS m/z (rel. int.): 258 $[\text{M}]^+$ (100), 240 $[\text{M} - \text{OH}]^+$ (69), 213 (30), 212 (29), 115 (24); IR $\nu_{\text{max}}^{\text{KBr}}$ cm^{-1} : 3227,

1758, 1610, 1572, 1460; $^1\text{H-NMR}$ ($\text{DMSO-}d_6$, 300 MHz) δ : 4.70 (2H, d, $J = 5.8$ Hz, 15-H), 5.80 (1H, t, $J = 5.8$ Hz, 15-OH), 6.70 (1H, d, $J = 3.4$ Hz, 13-H), 6.81 (1H, dd, $J = 2.4$, 8.6 Hz, 7-H), 7.07 (1H, d, $J = 8.6$ Hz, 8-H), 7.37 (1H, d, $J = 3.4$ Hz, 12-H), 7.47 (1H, s, 10-H), 7.84 (1H, d, $J = 2.4$ Hz, 5-H), 9.48 (1H, s, 6-OH); $^{13}\text{C-NMR}$ ($\text{DMSO-}d_6$, 75 MHz) δ : 56.4 (C-15), 110.9 (C-8), 111.0 (C-13), 111.1 (C-5), 115.5 (C-3), 117.0 (C-7), 122.4 (C-4), 123.3 (C-10), 124.3 (C-12), 146.5 (C-9), 149.5 (C-11), 153.9 (C-6), 162.1 (C-14), 168.9 (C-2).

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