Arch Pharm Res Vol 24, No 5, 416-417, 2001

Archives of Pharmacal Research
http://apr.psk.or.kr

A New Triterpene Lactone from the Roots of *Patrinia scabiosaefolia*

Mi Young Yang, Young Hae Choi, Hosup Yeo, and Jinwoong Kim

College of Pharmacy, Seoul National University, Seoul 151-742, Korea

(Received July 20, 2001)

A new triterpene lactone named patrinolide A (**1**) has been isolated from the roots of *Patrinia scabiosaefolia* (Valerianaceae). Its structure was determined to be 11β,21β-dihydroxy-3-oxooleanan-28,13β-olide on the basis of spectral analysis, including 2D-NMR techniques.

Key words: *Patrinia scabiosaefolia*, Valerianaceae, Lactone, Patrinolide, 11β,21β-dihydroxy-3-oxooleanan-28,13β-olide

INTRODUCTION

The roots of *Patrinia scabiosaefolia* Fischer (Valerianaceae) have been widely used in Korean traditional medicine for the treatment of inflammation and abscesses. It has been reported that the roots of this plant contain patrinoside, scopoletin, esculetin, and several triterpene glycosides (Taguchi and Endo, 1974; Choi and Woo, 1984; 1987). In this paper, we describe the isolation and structural elucidation of a new triterpene lactone, patrinolide A (**1**).

MATERIALS AND METHODS

The roots of *Patrinia scabiosaefolia* Fisher were purchased from Korea Export and Import Federation of Drugs, Seoul, Korea and identified by Dr Dae Suk Han, an emeritus professor of College of Pharmacy, Seoul National University. The 80% MeOH extract (212 g) of the dried roots of *P. scabiosaefolia* (1.2 kg) was suspended in water, and then partitioned with $CHCl_3$. The $CHCl_3$ extract (32 g) was subjected to column chromatography on silica gel with $CHCl_3$-MeOH gradient to give 7 fractions. Fr. 3 was submitted to repeated column chromatography over silica gel using *n*-hexane-$CHCl_3$-MeOH gradient system (5:5:1 to 1:1:1, v/v/v) to give fractions 8-13. Fr. 9 was subjected to Sephadex LH-20 column chromatography (*n*-hexane-acetone, 1:1) to yield compound **1** (10 mg).

Correspondence to: Jinwoong Kim, College of Pharmacy, Seoul National University, Shilim-Dong, Kwanak-Gu, San 56-1, Seoul 151-742, Korea
E-mail: jwkim@snu.ac.kr

Patrinolide A (**1**): White amorphous powder, mp. 246-249°C (decomposed); IR (KBr) cm^{-1}: 3500 (OH), 1737 (γ-lactone) and 1697 (C=O); EIMS m/z: 486 (M^+), 468; HR-EIMS m/z: 486.3354 (Calcd for $C_{30}H_{46}O_5$: 486.3345); ^{1}H-NMR (500 MHz, pyridine-d_5) δ: 0.86 (3H, s, H-25), 1.01 (3H, s, H-24), 1.14 (6H, s, H-30, H-23), 1.18 (3H, s, H-26), 1.29 (3H, s, H-29), 1.30 (3H, s, H-27), 3.37 (1H, br d, J=11.6 Hz, H-18), 3.92 (1H, dd, J=11.5, 4.0 Hz, H-21), 4.17 (1H, m, H-11); ^{13}C-NMR (125 MHz, pyridine-d_5) δ: 216.12 (C-3), 179.36 (C-28), 93.64 (C-13), 73.01 (C-21), 66.88 (C-11), 54.63 (C-5), 48.64 (C-9), 47.34 (C-4), 45.94 (C-17), 42.97 (C-14), 42.57 (C-8), 42.34 (C-18), 39.62 (C-1), 37.51 (C-20), 37.33 (C-22), 37.05 (C-19), 36.66 (C-10), 34.27 (C-2), 33.05 (C-7), 30.06 (C-29), 29.48 (C-12), 27.84 (C-15), 26.57 (C-23), 22.57 (C-16), 21.20 (C-24), 19.21 (C-6), 19.01 (C-26), 18.34 (C-27), 18.03 (C-30), 15.93 (C-25).

RESULTS AND DISCUSSION

Patrinolide A (**1**) was obtained as a white amorphous powder. The molecular formula $C_{30}H_{46}O_5$ (M^+ *m/z*: 486.3354, Calcd 486.3345) was determined by high-resolution MS spectrum. Its IR spectrum displayed absorption bands at 3500 (OH), 1737 (γ-lactone) and 1697 (C=O) cm^{-1}. The ^{1}H-NMR spectrum of **1** showed seven tertiary methyl (δ 0.86-1.30) and two carbinolic methine [δ 3.92 (1H, dd, *J*=11.5, 4.0 Hz) and δ 4.17 (1H, m)] signals, which suggested that **1** was an oleanane-type triterpene with two hydroxyl groups. In its ^{13}C-NMR spectrum, the characteristic peaks at δ 216.12, 179.36 and 93.64 implied **1** was 3-oxooleanan-28,13β-olide (Poehlane *et al.*, 1987). The HMBC spectrum of **1** showed cross-peaks

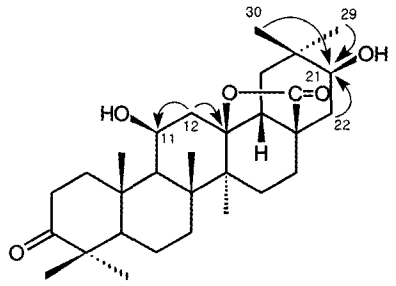

Fig. 1. ^{1}H-^{13}C long-range correlations observed from the HMBC spectrum of **1**. Most protons are omitted for clarity.

of correlation from δ_H 1.97 (H_2-12) to δ_C 66.88 (C-11), and from δ_H 1.14 (H_3-30), 1.29 (H_3-29) and 2.31 (H_2-22) to δ_C 73.01 (C-21), indicating the presence of hydroxyl groups in the position of C-11 and C-21. The configuration of hydroxyl group at C-11 was determined to be β-form on the basis of $J_{10,11}$ (3.2 Hz) in the decoupling experiment (CD_3OD). Also, the coupling constant of $J_{21,22}$ suggested the hydroxyl group at C-21 had β configuration. From all the above data, the structure of **1** was elucidated as 11β,21β-dihydroxy-3-oxooleanan-28,13β-olide.

ACKNOWLEDGEMENTS

This work was supported in part by the Research Institute of Pharmaceutical Sciences, Seoul National University.

REFERENCES

Choi J. S., Woo W. S., Coumarins and triterpenoid glycosides from the roots of *Patrinia scabiosaefolia*. *Arch. Pharm. Res.*, 7, 121-126 (1984).

Choi J. S., Woo W. S., Triterpenoid glycosides from the roots of *Patrinia scabiosaefolia*. *Planta Med.*, 53, 62-65 (1987).

Poehland B. L., Carte B. K., Francis T. A., Hyland L. J., Allaudeen H. S., Troupe N., *In vitro* antiviral activity of dammar resin triterpenoids. *J. Nat. Prod.*, 50, 706-713 (1987).

Taguchi H., Endo T., A new iridoid glycoside from *Patrinia scabiosaefolia*. *Chem. Pharm. Bull.*, 22, 1935-1937 (1974).