Phytochemistry, Vol. 26, No. 10, pp. 2849–2850, 1987.
Printed in Great Britain.

0031–9422/87 \$3.00 + 0.00

A POLYACETYLENIC COMPOUND FROM *PANAX GINSENG* ROOTS

SANG CHUL SHIM*, SUK-KU CHANG, CHAN WOO HUR and CHANG KEW KIM

*Korea Advanced Institute of Science and Technology, P.O. Box 150, Chongyangni, Seoul 131 Korea; Pacific R & D Center, 686-5, Sindaebang-Dong, Dongjak-ku, Seoul 151 Korea

(*Revised received* 10 *March* 1987)

Key Word Index—*Panax ginseng*; Araliaceae; C_{17} polyacetylene; heptadeca-1,8-dien-4,6-diyn-3,10-diol.

Abstract—A new polyacetylenic compound was isolated from Korean ginseng roots. The structure was determined to be heptadeca-1,8-dien-4,6-diyn-3,10-diol by spectral methods.

INTRODUCTION

Recently, it was reported [1, 2] that the petrol fraction extracted from Korean ginseng roots inhibits the growth of murine leukema L5178Y and murine Sarcoma 180 cells *in vitro*, and also inhibits DNA, RNA and protein synthesis in murine ascitic Sarcoma 180 cells *in vitro*. The petrol–diethyl ether extracts from ginseng roots contain many compounds, and a polyacetylenic compound is one of the major components.

The first polyacetylenic compound from *Panax ginseng* was isolated by Takahashi *et al.* [3, 4]. Other polyacetylenic compounds were also isolated and characterized afterwards by Wrobel *et al.* [5–7] and Shim *et al.* [8]. A few more new polyacetylenic compounds were detected in the HPLC chromatogram of the etheral extracts of ginseng. However, the isolation of these new polyacetylenic compounds from ginseng was not pursued due to their thermal and photochemical instability and the difficulty in isolating sufficient quantities for characterization. We now report the isolation and characterization of a new polyacetylenic compound from fresh ginseng roots.

RESULTS AND DISCUSSION

A new polyacetylenic compound ($C_{17}H_{24}O_2$) was isolated from an ethereal fraction of the methanolic extracts of *Panax ginseng*. The UV spectrum of the separated component showed λ_{max} at 283, 268, 253, 238 and 226 nm with band spacing of about 2000 cm^{-1} indicating that the component is a polyacetylenic compound having a diyn-ene chromophore with two conjugated triple bonds and one double bond.

The molecular skeleton of **1** was easily recognized by its ^{13}C NMR spectrum (50.32 MHz, $CDCl_3$). The proton wide band decoupled spectrum of **1** showed the typical aliphatic methylene carbons at δ 23.3, 32.5, 30.1, 29.9, 25.9 and 37.6, the terminal methyl carbon of the straight aliphatic chain at 14.7, the two carbons of the terminal vinyl group at 110.7 and 136.8, allylic carbon to the terminal vinyl group at 64.3, two carbons of the internal vinyl group at 108.8 and 150.6 and the allylic carbon to the internal vinyl group at 72.8. The resonance peaks of the quarternary carbons in the conjugated triple bonds were observed at δ81.3, 73.7 and 71.0 but they were not definitely assigned because only three were observed instead of the anticipated four, one being superimposed with a solvent peak.

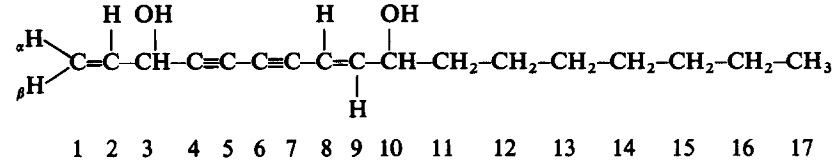
The ^1H NMR spectrum (200 MHz, $CDCl_3$) of **1** showed the typical spin system of a terminal vinyl group (between δ5.16–5.97), protons of an internal double bond (between 5.66–6.32), protons of a secondary hydroxyl group at 4.90 and 4.11, methylene protons of a straight hydrocarbon chain at 1.39 and the corresponding terminal methyl group protons at 0.81.

The mass spectrum of **1** determined by EI did not show the M^+ at m/z 260 due to its easy fragmentation, but showed a fragment ion peak at m/z 161 which was probably due to allylic fission. The elemental analysis data of **1** were consistent with the molecular formula, $C_{17}H_{24}O_2$.

From these results, compound **1** is determined to be heptadeca-1,8-dien-4,6-diyn-3,10-diol, a new polyacetylenic compound among the C_{17} naturally occurring polyacetylenes in Korean ginseng roots.

EXPERIMENTAL

Isolation of heptadeca-1,8-dien-4,6-diyn-3,10-diol. Fresh Korean ginseng roots (*Panax ginseng* C. A. Meyer; 20 kg) were finely crushed up and extracted with MeOH. The MeOH extracts were partitioned with petrol–Et_2O (4:1). The petrol–Et_2O layers were collected and the solvent evapd. The crude oily mixture (100 g) was dissolved in *n*-hexane and Et_2O. Stepwise gradient elution from a silica gel column with *n*-hexane–Et_2O (2:1–1:2) gave a fraction containing a new polyacetylenic compound. To isolate the polyacetylene, semi-prep. HPLC was carried out under the following conditions; column: Lichroprep Si 60 (40–63 μm) Lobar Prepacked Column, solvent: *n*-hexane–Et_2O (3:1), flow rate: 5.0 ml/min, detector: UV (254 nm). Finally, to isolate the pure polyacetylenic compound, prep. HPLC was performed under the following conditions; column: prep-LiChrosorb CN (10 mm i.d. x 25 cm), solvent: *n*-hexane–Et_2O (2:1), flow rate: 4.0 ml/min, detector: UV (254 nm). The R_t value (min) was 9.5. The polyacetylene was collected in bottles immersed in a dry ice-acetone bath and covered with aluminium foil to shield it from light. The purity of the separated fraction was rechecked by analytical HPLC. For spectroscopic measurements, the collected fraction was concentrated by evaporation in a stream of N_2.



1

Residual solvents were removed by a rotary vacuum evaporator.

Heptadeca-1,8-*dien*-4,6-*diyn*-3,10-*diol* (1). ^{1}H NMR (200 MHz, $CDCl_3$, TMS as int. st.): δ6.27 (1H, *dd*, $J = 15.9$, 5.6 Hz, C-9), 5.89 (1H, *ddd*, $J = 17.2, 9.6, 5.4$ Hz, C-2), 5.70 (1H, *d*, $J = 15.9$ Hz, C-8), 5.41 (1H, *dd*, $J = 17.2$, 2.1 Hz, C-1), 5.19 (1H, *dd*, $J = 9.6$, 2.1 Hz, C-1), 4.91 (1H, *d*, $J = 5.4$ Hz, C-3), 4.12 (1H, *dt*, $J = 5.6$, 2.0 Hz, C-10), 1.39 (12H, *m*, $-(CH_2)_6-$), 0.81 (3H, *t*, C-17); UV λ_{max}^{MeOH} nm: 283, 268, 253, 238, 226; IR ν_{max}^{NaCl} cm^{-1}: 3356 (–OH), 2234 (C≡C), 955 (CH=CH); ^{13}C NMR (50.32 MHz, $CDCl_3$): δ150.6 (C-9), 136.8 (C-2), 117.8 (C-1), 108.8 (C-8), 81.3 (C-4), 73.7 (C-5), 72.8 (C-10), 71.0 (C-6), 64.3 (C-3), 37.6 (C-11), 32.5 (C-16), 30.1 (C-14), 29.9 (C-13), 25.9 (C-12), 23.3 (C-15), 14.7 (C-17). (Found: C, 78.18; H, 9.34. $C_{17}H_{24}O_2$ requires C, 78.47: H, 9.23%).

Acknowledgement—This investigation was supported by the Korea Advanced Institute of Science and Technology, and Pacific R & D center.

REFERENCES

1. Hwang, W. I. and Cha, S. M. (1978) in *Proceedings of the Second International Ginseng Symposium* p. 43. Seoul.
2. Yun, Y. S., Lee, Se Y., Kim, B. S. and Yun, T. K. (1980) *J. Korean Biochem.* **13**, 203.
3. Takahashi, M. and Yoshikura, M. (1964) *J. Pharm. Soc. Jpn* **84**, 752.
4. Takahashi, M. and Yoshikura, M. (1964) *J. Pharm. Soc. Jpn* **84**, 757.
5. Wrobel, J. T., Dabrowski, Z., Gielzynska, H. K., Iwanow, A., Kabzinska, K., Poplawski, J. and Ruszkowska, J. (1973) *Tluszcze Srodki Piorace, Kosmet.* **17**, 63.
6. Poplawski, J., Wrobel, J. T. and Glinka, T. (1980) *Phytochemistry* **19**, 1539.
7. Dabrowski, Z., Wrobel, J. T. and Wojtasiewicz, K. (1980) *Phytochemistry* **19**, 2464.
8. Shim, S. C., Koh, H. Y. and Han, B. H. (1983) *Phytochemistry* **22**, 1817.

Phytochemistry, Vol. 26, No. 10, pp. 2850–2852, 1987.
Printed in Great Britain.

0031-9422/87 $3.00+0.00
Pergamon Journals Ltd.

ACETYLENES FROM THE CALLUS OF *PANAX GINSENG*

YASUO FUJIMOTO* and MITSURU SATOH†

The Institute of Physical and Chemical Research, Wako, Saitama 351–01, Japan

(*Revised received* 27 *February* 1987)

Key Word Index—*Panax ginseng*; Araliaceae; C_{17}-polyacetylenes; callus; anticancer activity.

Abstract—Two new polyacetylenes were isolated from dried callus of *Panax ginseng*. The structures of the polyacetylenes were confirmed as heptadeca-3-oxo-4,6-diyne-9,10-diol and its dihydro derivative by their IR, ^{1}H NMR, ^{13}C NMR and mass spectra, and some chemical reactions. The new acetylenes exhibited growth inhibition against Yoshida sarcoma cells in tissue culture.

INTRODUCTION

From ancient times *Panax ginseng* C. A. Mayer has been considered as one of the most valuable drugs to be used in Korea, China and Japan. Studies on the constituents of *P. ginseng* have been mainly focused on the ginseng saponins. Since the anticancer activity of petrol extracts of the roots of *P. giseng* was found [1], the lipophilic portion of this plant has been extensively investigated. Several groups have isolated polyacetylene compounds, however, it has not been proved that the polyacetylenes in the plant are responsible for the growth inhibition of cancer cells [2].

---

*Author to whom correspondence should be addressed.

†Visiting scientist from Showa Pharmaceutical College, July 1985–March 1986.