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A Pyrrolo-pyrimidine Alkaloid from *Glycyrrhiza uralensis*

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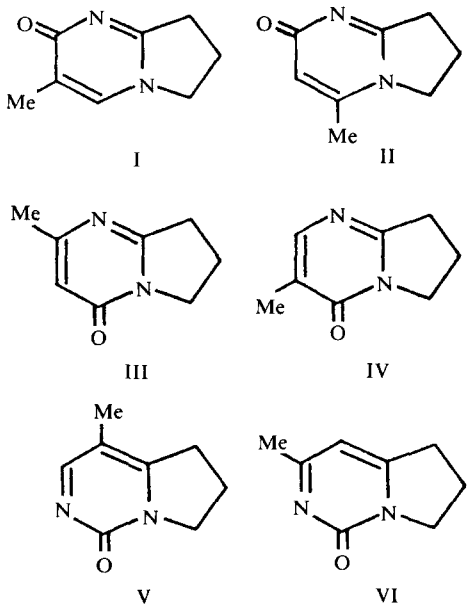
Abstract□An alkaloid was isolated from the roots of *Glycyrrhiza uralensis* Fisch. It was identified as 3-methyl-6,7,8-trihydro-pyrrolo[1,2-a]pyrimidin-2-one(I) by spectral analysis. The compound is first found in the plant kingdom.

Keywords□*Glycyrrhiza uralensis,* pyrrolo[1,2-a]pyrimidine alkaloid, licorice.

In a previous paper[1], we elucidated the structure of two quinoline alkaloids isolated from the roots of *Glycyrrhiza uralensis* Fischer et DC, first reporting the alkaloid isolation from *Glycyrrhiza* species. The present paper describes the characterization of another alkaloid isolated from the licorice roots.

The alkaloid showed an UV absorption maximum at 266 nm. Its IR spectrum revealed the presence of olefinic proton at 3090 and 860 cm^{-1} and α, β-unsaturated carbonyl group at 1660 and 1545 cm^{-1}. The molecular formula of the alkaloid was determined as $C_8H_{10}N_2O$ by mass (M^+ at *m/z* 150) and ^{13}C-NMR spectra. The eight carbons were assigned by an attached proton test to one CH_3, three CH_2, one CH, two C and one C=O. In its ^1H-NMR spectrum, the methyl group was found at δ 2.48(s), the three methylenes were at δ 2.60(m), 2.69(t) and 4.00(t), and the olefinic proton was at δ 7.52(s). From these data, we can draw six kinds (I-VI) of postulated structure as following (Scheme 1).



Scheme 1.

As shown in Fig. 1, irradation of the methyl group at δ 2.48 yielded NOE at the olefinic proton of δ 7.20(2.2%). On irradation of the olefinic proton at δ 7.20, NOEs were oserved at the methyl group of δ 2.48 (0.7%) and at the methylene of δ 4.00 (1.2%). The results unambiguously indicated the structure of the alkaloid to be I, 3-methyl-6, 7, 8-trihydro-pyrrolo[1, 2-a]pyrimidin-2-one. The compound is first found in the plant kingdom, though it was already synthesized by Kökosi, *et al.*[2] who found its antianginal and digitalis-like activities.

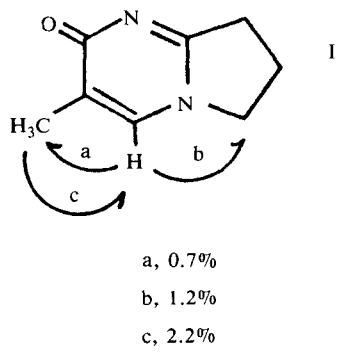


Fig. 1. Nuclear overhause effect of an alkaloid isolated from the roots of *Glycyrrhiza uralensis*. Irradiated at δ 2.48 and 7.20.

EXPERIMENTAL

Isolation of the alkaloid

An alkaloidal fraction of the licorice roots was prepared by the previous method[1], and was subjected to column chromatography over silica gel (E. Merck, type 60, no.7734) using chloroform and then chloroform/methanol (50:1 → 20:1) to afford fractions A, B and C, respectively. An alkaloid was isolated from Fr. C by repeated chromatography over silica gel (E. Merck, type 60, no.7729) utilizing two solvent systems of chloroform/ethyl ether (1:1) and then chloroform/methanol (20:1). Rf: 0.3 ($CHCl_3$/MeOH = 20:1). M.P.:224°C (Lit.[2] 242°C). UV λ_{max}:266 nm. IR ν_{max}:3090 (C=CH), 1665 (conjugated C=O), 1545, 1190, 1100, 950, 860 cm^{-1}. MS *m/z* (%):EIMS, 150 (M^+, 35.6), 135 (M-CH_3, 100), 105 (18.2); SIMS, 151 ($M^+ + 1$, 100). ^{1}H-NMR (δ ppm, $CDCl_3$):2.48 (3H, s, CH_3), 2.60 (2H, m, 6-CH_2), 2.69 (2H, t, 8-CH_2), 4.00 (2H, t, 7-CH_2), 7.52 (1H, s, olefine). ^{13}C-NMR (δ ppm, $CDCl_3$): 26.5 (CH_3), 22.7 (7-CH_2), 26.1 (8-CH_2), 44.8 (6-CH_2), 119.0 (4-CH_2), 146.6 (3-C), 155.1 (9-C).

Instrumental

Mp was determined on a Mitamura-Ricken heating block and uncorrected. A recording spectrophotometer, Gilford type 2600 was used for the measurement of UV spectrum. IR absorption spectrum was obtained in KBr pellet on a Perkin-Elmer model 283B spectrophotometer. NMR spectra were taken at 25°C using TMS as an internal standard on a Nicolet NT-360 spectrometer. EIMS and SIMS spectra were otained on a Hewlett-Packard GC/MS spectrometer (type 5985B) and on a Hitachi M-80 high resolution mass spectrometer, respectively.

ACKNOWLEDGEMENT

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