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OREACONINE — A NEW ALKALOID FROM *Aconitum orientale*

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Continuing an investigation of the alkaloids of *Aconitum orientale* growing on Turkish territory, with the aid of various methods of electron-impact (EI) mass spectrometry and secondary-ion mass spectrometry (LSIMS), together with methyllappaconitine, having M^+ 682, we have detected the presence in the roots of the plant of another base, with M^+ 682, $C_{37}H_{50}N_2O_{10}$ (**1**). Isolated with the aid of column chromatography and called by us oreaconine (**1**), it formed a white amorphous powder readily soluble in the usual organic solvents.

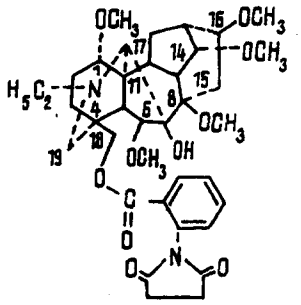
Oreaconine gave a crystalline perchlorate with mp 157—159°C (from MeOH, foaming). The IR spectrum of the perchlorate of (**1**) (tablet with KBr) contained absorption bands at (cm^{-1}) 3500 (OH group), 1720, 1260 (ester group), 1605, 1585, 770 (benzene ring), and 1100 (ether C—O bond). The PMR spectrum of base (**1**) (100 MHz, CD_3OD, 0 — HMDS, δ scale, ppm) showed signals from a N-ethyl group (0.98, 3H, t, J = 7.5 Hz) and five methoxy groups (3.20, 3H, s; 3.28, 6H, s; 3.38, 6H, s).

In the spectrum of the perchlorate of (**1**) taken under the same conditions, signals of methoxy groups were observed at (ppm) 3.30, 3.33, 3.34, 3.35, and 3.37. In addition to those shown in the spectrum of (**1**), which was similar to that of lycaconitine [2], there was a signal at 2.84 ppm in the form of a four-proton singlet, and, between 7.25 and 8.09 ppm, signals from four aromatic protons, due to the presence of a succinimidylanthranilic acid (SAA) residue. The EI mass spectrum of (**1**) had the peaks of ions with m/z 682 (M^+ 2.0), 681(1.0), 667(3.9), 651($C_{36}H_{47}N_2O_9$; 100), 650(47), 635(31), 619(20), 589(13), 202($C_{11}H_8NO_3$; 50), 174(17), 146(24).

What has been said above and also the results of a comparison of the mass spectrum of (**1**) with those of septentrionine [2], deacetylambiguine [3], peregrine [4], and the information givem in [5—8] showed in combination that oreaconine belonged to the C_{19}-diterpene alkaloids of the lycoctonine type with the position of one of the methoxy groups at C-1 and the SAA residue at C-18, and made it possible to assume that the sole hydroxyl and the second methoxy group were present at C-7 and C-8, respectively.

In the weak field of the PMR spectrum of (**1**) at 3.45 ppm there was a one-proton signal in the form of a doublet of doublets with J_1 = 4.5 Hz and J_2 = 1.0 Hz, which is characteristic for H-14β geminal to a methoxy group [9], and at 3.62 ppm a 1H signal in the form of a broadened singlet, which is characteristic for H-6α geminal to a methoxy group [3].

In view of the combined presence in *A. orientale* of (**1**) and lycoctonine, anthranoyllycoctonine, methyllycaconitine, and lycaconitine [1], which, like the overwhelming majority of alkaloids of the lycoctonine type, have an α-oriented substituent at C-1 and a substituent with the β-configuration at C-16, and taking biogenetic considerations into count, on the basis of the facts given above it is possible to propose for oreaconine the most probable structure (**1**).



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