# THE STRUCTURE OF VERALOMINE

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We have previously [1] reported the isolation from the combined bases of the epigeal part of *Veratrum lobelianum* of an alkaloid with mp 275-277°C, $[\alpha]_D$ −54.11°. This new base, $C_{33}H_{53}NO_6$, we have called veralomine (I). The base has also been isolated from the combined alkaloids of the epigeal part of the same plant. IR spectrum of (I): $\nu_{max}$ 3400 $cm^{-1}$, 1100-1010 (OH). It forms a O, N-pentaacetyl derivative (II) with mp 201-202°C, $[\alpha]_D$ −59.7° ($CHCl_3$ here in the other determinations). IR spectrum of (II); $\nu_{max}$ 1740, 1230 $cm^{-1}$ (O-acetyl), 1630 $cm^{-1}$ (N-acetyl).

Two aglycones were isolated from the products of the acid hydrolysis of (I): $C_{27}H_{43}NO$ with mp 174-175°C, $[\alpha]_D$ −53.23°, and $C_{27}H_{41}N$ with mp 175-178°C, $[\alpha]_D$ −49,5°, which we have called veralomidine (III) and veralomidene (IV), and also D-glucose (paper chromatography). IR spectrum of (III): $\nu_{max}$ 3250 $cm^{-1}$ (OH), 3035, 1065 $cm^{-1}$ ($\Delta^5$, 3β-OH) [2]. The aglycone (III) gave a digitonide (3β-OH) and belongs to the typical steroid alkaloids. The acetylation of (III) led to the formation of the O,N-diacetyl derivative (V) with mp 186-188°C, $[\alpha]_D$ −36,7°. Its IR spectrum: $\nu_{max}$ 1740, 1240 $cm^{-1}$ (O-acetyl), 1640 $cm^{-1}$ (N-acetyl). The partial saponification of (V) gave N-acetylveralomidine (VI) with mp 198-199°C. IR spectrum of (VI): $\nu_{max}$ 1620 $cm^{-1}$ (N-acetyl), 3365 $cm^{-1}$ (OH).

The Adams hydrogenation of (III) in ethanol led to dihydroveralomidine (VII) with mp 216-218°C, $[\alpha]_D$ −32°, and its hydrogenation in glacial acetic acid led to tetrahydroveralomidine with mp 213-215°C, $[\alpha]_D$ + 9°.

Veralomidine forms a nitroso derivative (VIII) with mp 202-205°C (decomp.). The UV spectrum of (VIII) [238, 290 nm (log ε 3.98, 3.72)] is similar to that of the nitroso derivative of veralinine [3].

The NMR spectrum of (III) ($CDCl_3$ on a JNM-4H-100 MHz instrument with HMDS, δ scale) shows the resonance signals from two tertiary methyl groups at 0.99 and 0.78 ppm, doublets at 0.76 ppm (3H, 21-$CH_3$), and 0.92 ppm (3H, 27-$CH_3$), and multiplets at 3.45 ppm (CH—OH) and 5.32 ppm (vinyl protons at $C_6$ and $C_{12}$) [3, 4].

The mass-spectrometric decomposition of (III) took place similarly to that of veralkamine and veralinine, i.e., it showed the main peaks of ions with m/e 98 (100%), 380 (M − 17), 382 (M − 15), and 397 ($M^+$).

On the basis of the results presented, veralomidine belongs to the type of veralkamine and has the veralinine skeleton [3]. However, veralomidine is not identical with veralinine and apparently differs from it by the configuration of the $C_{17}$ asymmetric center.

The IR spectrum of veralomidene (IV) lacks the absorption band of a hydroxy group. The UV spectrum has $\lambda_{max}$ 232, 238, 248 nm (log ε 4.26, 4.30, 4.12), which is characteristic for a heteroannular diene [5].

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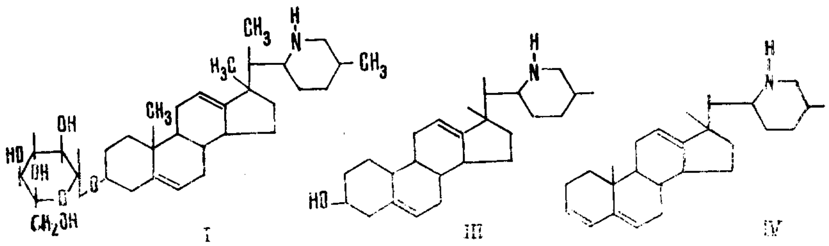
Consequently, in the hydrolysis of (I), in addition to the splitting off of the D-glucose a molecule of water splits off at the expense of the OH group at $C_3$ and H at $C_4$. Such cases are observed in the hydrolysis of a number of glycoalkaloids [6], as was confirmed by the formation of (IV) when (III) was heated in 10% sulfuric acid.

The facts given above show that the most probable structures of (III) and (IV) are:



I III IV

The results of a comparison of molecular rotations showed that in veralomine, according to Klyne's rule [7] the D-glucose is attached to the hydroxy group at $C_3$ of veralmidine by a β-glycosidic link. Hence veralomine has the structure of veralomidine 3β-D-glucopyranoside (I).

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