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THE REVISED STRUCTURE OF VERAMARINE, AN ALKALOID FROM Veratrum album ssp.Lobelianum

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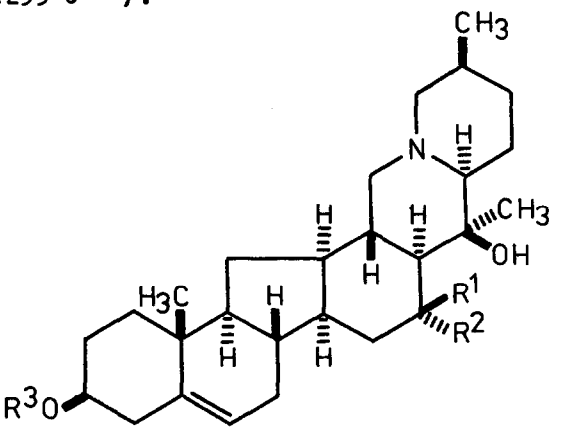
In previous papers[1,2] we presented the spectral evidence enabling us to formulate the structure of veramarine, the minor alkaloid from Veratrum album subsp. Lobelianum /BERN./ Suessenguth as I. The spatial arrangement of this base was supported by analogy and biogenetic consideration of the C-nor-D-homo steroidal type of alkaloids. Feeling the need for more substantial proof of this proposal, we turned our attention to a single- crystal X-ray analysis. Since veramarine is amorphous[3], we prepared its well crystallizing acetate/ III, $C_{29}H_{45}NO_4$, m.p.255°C [1] /.

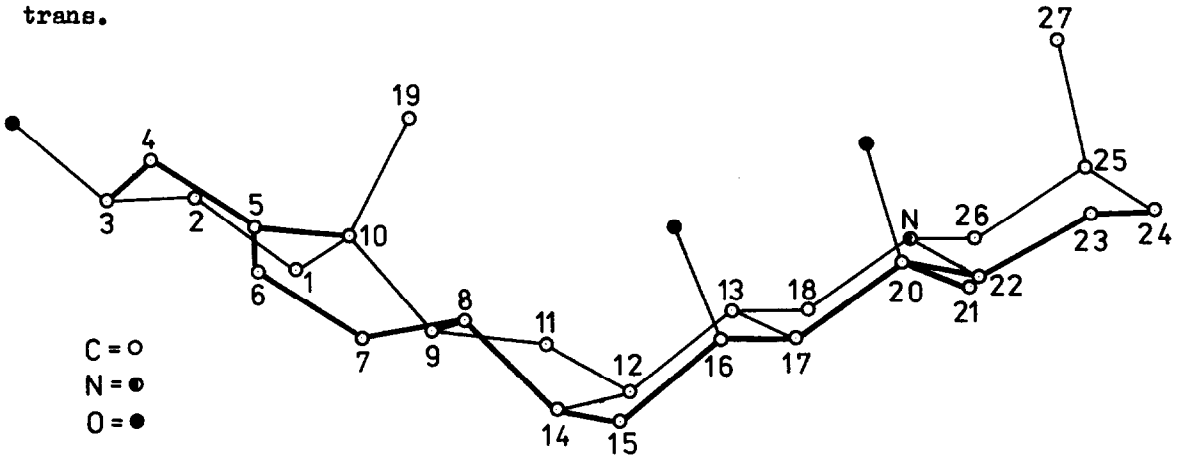
	R^1	R^2	R^3
I	H	OH	H
II	OH	H	H
III	OH	H	CH_3CO



This compound crystallized from ether in prismatic form. The crystal belongs to the orthorhombic system, space group $P2_1\ 2_1\ 2_1$ in a cell of dimensions a = 6.342, b = 20.961, c = 19.809 Å, Z = 4. The three-dimensional diffraction data were collected with a Syntex $P2_1$ 4-circle diffractometer, using θ-2θ scan technique and graphite monochromated Cu K_α radation. A total

of 2085 independent structure factors were evaluated for the analysis. The positions of nonhydrogen atoms were determined by direct methods. The atomic parameters were refined by the block-diagonal least-squares to a R-value of 4.7 % with 1501 observed reflexions.

The X-ray analysis confirmed the previously proposed structure except of the C_{16}-OH group, which is axial as shown in II. The absolute configuration of the molecule is as in the similar alkaloid verticinone methobromide[4]. The ring juncture is A/B trans, B/C trans, C/D cis, D/E trans and E/F trans.



The configurations at other chiral centres were settled as C_3-OH equatorial, C_{10}-Me axial, C_{20}-OH axial, C_{20}-Me equatorial C_{25}-Me axial.

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