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THE STRUCTURE OF OCHOTENSINE AND OCHOTENSIMINE

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The alkaloids ochotensine and ochotensimine were isolated from Corydalis ochotensis by Manske (1), who showed that ochotensimine is simply the O-methyl ether of the phenolic base ochotensine. Structure I, incorporating a novel benzylisoquinoline skeleton, has been proposed for ochotensimine mainly on the basis of NMR data (2), and we now report an X-ray analysis of ochotensine methiodide, which confirms ochotensimine as I, and establishes the structure of ochotensine as II.

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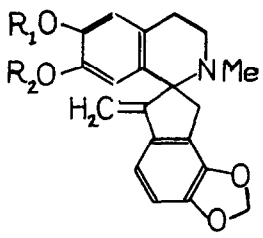

I, $R_1 = R_2 = Me$

II, $R_1 = H$, $R_2 = Me$

Crystals of ochotensine methiodide, $C_{21}H_{21}O_4N.CH_3I$, from methanol, have m.p. 215°, and are tetragonal, $\underline{a}$ = 12.65 ± 0.03, $\underline{c}$ = 25.89 ± 0.08 Å, $\underline{Z}$ = 8, $\underline{D}_m$ = 1.61, $\underline{D}_x$ = 1.58 g cm^{-3}, space group $\underline{P}4_12_12$ or $\underline{P}4_32_12$. The intensities of 847 independent reflexions (668 observed) were measured visually, the iodide ion position was determined from the three-dimensional Patterson function, and all the carbon, nitrogen and oxygen atoms were located from three successive three-dimensional electron-density distributions. The positional and anisotropic thermal parameters were then refined by eight cycles of block-diagonal least-squares, the final $\underline{R}$-value being 0.09 for the 668 observed reflexions. Sections of a final three-dimensional electron-density distribution, taken through the atomic centers parallel to (100), are shown in Fig. 1, together with a drawing of the molecule. The results prove structure II for ochotensine, and hence I for ochotensimine.

The computations were performed on the IBM 7040 Computer with our own programs, and we thank the staff of the University of British Columbia Computing Center for assistance, and the National Research Council of Canada for financial support.

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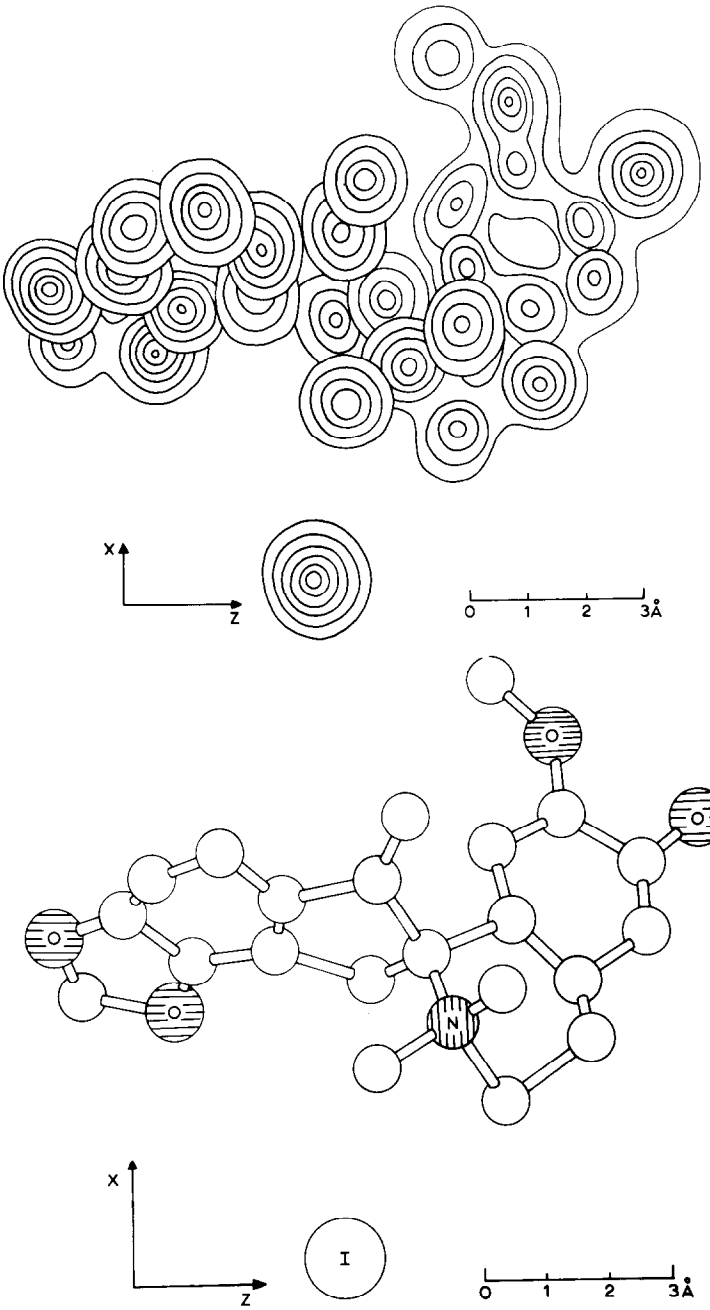
1. R.H.F. Manske, Can. J. Research B, 18, 75 (1940).

2. S. McLean and M.-S. Lin, Tetrahedron Letters, 3819 (1964).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