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X-RAY STRUCTURE DETERMINATION OF DIHYDROTELEOCIDIN B MONOBROMOACETATE.

N.Sakabe, H.Harada, Y.Hirata.
Chemical Institute, Faculty of Science,
Nagoya University, Nagoya, Japan.
and
Y.Tomiie, I.Nitta.
Faculty of Science, Kwansei Gakuin University,
Nishinomiya, Japan.

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As discussed in the preceding paper (1), a structure containing a substituted indole nucleus with a nine-membered lactam ring has been suggested for dihydroteleocidin B, which was derived from teleocidin B, a toxic principle of mycelia of some Streptomyces. In parallel with these chemical investigations, the X-ray crystallographic studies were carried out for elucidation and confirmation of the complete structure of this substance, and the results are presented in this communication.

Treatment of dihydroteleocidin B with monobromoacetyl bromide afforded dihydroteleocidin B monobromoacetate, m.p. 214-216°C, $C_{30}H_{44}O_3N_3Br$, U.V. $\lambda_{max.}^{MeOH}$ 232 mμ. (log ε = 4.48), 287 mμ. (log ε = 3.91), I.R. max. 1742, 1655, 1595, 1300, 1180, 1160 cm^{-1}. The crystal is orthorhombic with the unit cell of the dimensions, a = 14.50, b = 26.60, c = 7.39 A, the space group being $P2_12_12_1$, and there are four molecules per unit cell.

The intensities of the three-dimensional reflections were measured visually from integrating Weisenberg photographs around a and c axes taken with filtered Cu Kα radiation. Relative values of the observed structure factors of 3546 reflections were converted into absolute scale by Wilson's method (2).

The position of the bromine atom was determined by the three-

dimensional Pattersen function. Three-dimensional minimum function method (3) was carried out for the elucidation of the positions of light atoms. The structure thus obtained was refined by the three-dimensional Fourier synthesis and the least-squares method. The R factor is 16.4 per cent at the present stage.

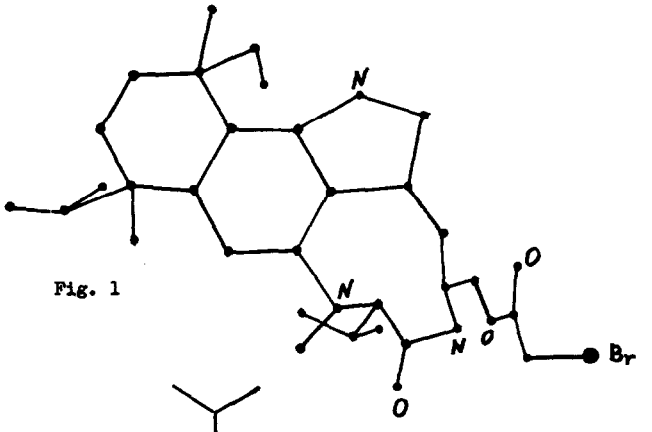

Fig. 1

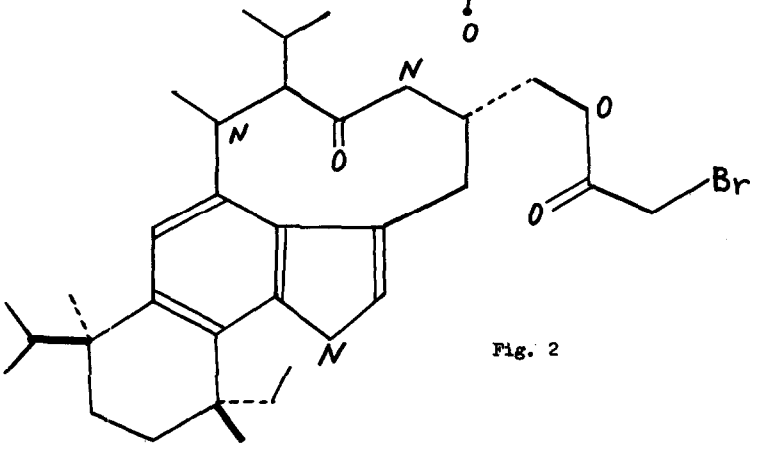

Fig. 2

The molecular framework projected along the c axis is shown in Fig. 1, and the complete chemical formula of dihydroteleocidin B monobromoacetate is illustrated in Fig. 2.

The calculations were performed on the NEAC-2206 electronic

computer using our programs. The authors are grateful to Takeda Chemical Industries, Ltd. for making the computer available, and are indebted to the National Institute of Health which supported this work through Grants RG-7969 and GM-7969.

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