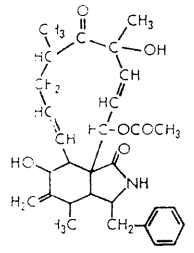
Structure of Zygosporin A: *X*-Ray Analysis of Isozygosporin A *p*-Bromobenzoate

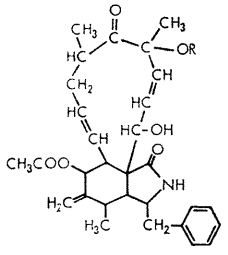
By Y. TSUKUDA, M. MATSUMOTO, H. MINATO, and H. KOYAMA*

(*Shionogi Research Laboratory, Shionogi & Co., Ltd., Fukushima-ku, Osaka, Japan*)

IN a previous communication[1] a new antibiotic compound, Zygosporin A, was reported, with the empirical formula $C_{30}H_{37}O_6N$. From an *X*-ray structure analysis of isozygosporin A *p*-bromobenzoate (III) and various chemical information, Minato assigned[2] the formulae (I) to zygosporin A and (II) to isozygosporin A.



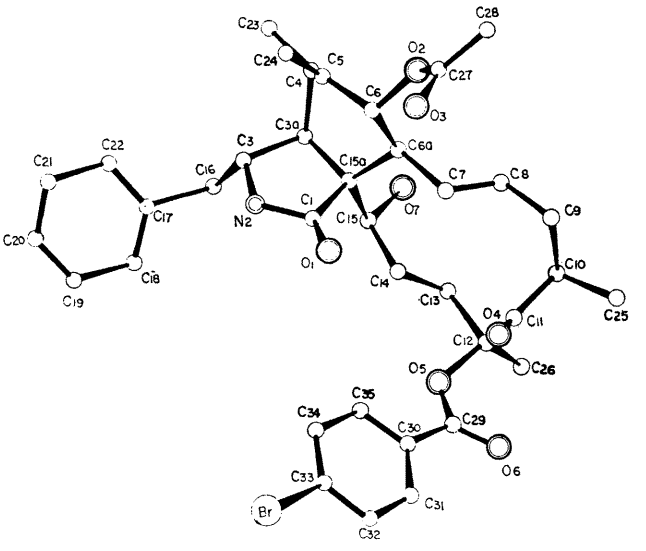
(I)



(II) R = H
(III) R = -CO-C$_6$H$_4$-Br

We report the crystal structure of isozygosporin A *p*-bromobenzoate elucidated by three-dimensional *X*-ray structure analysis. The compound was recrystallised from isopropyl alcohol at room temperature. Crystal data: $C_{37}H_{40}O_7NBr$, $x\,C_3H_8O$ ($x = ca.\ \frac{1}{2}$) $M = 751$, m.p. 242—245°, orthorhombic, $a = 22{\cdot}535 \pm 0{\cdot}004$, $b = 12{\cdot}332 \pm 0{\cdot}002$, $c = 13{\cdot}917 \pm 0{\cdot}002$ Å, $U = 3867$ Å^3, $D_m = 1{\cdot}281$, $Z = 4$, $D_c = 1{\cdot}289$, space group, $P2_12_12_1$.

Three-dimensional intensity data were collected on a Hilger and Watts automatic four-circle diffractometer, with a scintillation counter, Mo-K_α radiation (Zr-filter θ and pulse-height analyser), and an θ—2θ scanning method. 3606 independent reflexions were recorded, of which 2067, with intensities significantly above background, were used. The structure was solved by heavy-atom and three-dimensional Fourier methods, and refined by least-squares calculations, to R 9·1%. The overall geometry of the molecule is shown in the Figure.



FIGURE

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[1] S. Hayakawa, T. Matsushima, T. Kimura, H. Minato, and K. Katagiri, *J. Antibiotics*, 1968, **21**, 523.
[2] H. Minato and M. Matsumoto, *J. Chem. Soc.* (*C*), to be published.