STUDIES ON A NEW ANTIBIOTIC
FR-900109
2. X-RAY STRUCTURE DETERMINATION OF FR-900109 p-BROMOPHENYL ESTER

SHIGETAKA KODA and YUKIYOSHI MORIMOTO
Central Research Laboratories

MICHIO YAMASHITA, TADAAKI KOMORI and HIROSHI IMANAKA
Fermentation Research Laboratories
Fujisawa Pharmaceutical Co., Ltd.
1-6, 2-chome, Kashima, Yodogawa-ku, Osaka 532, Japan
(Received for publication February 24, 1983)

A new antibiotic called FR-900109 was obtained from streptomycetes identified as Streptomyces prunicolor and its producing strain, fermentation, isolation procedures, chemical and biological properties have been reported in a previous paper1). In this paper, the crystal structure of FR-900109 p-bromophenyl ester will be described.

Prismatic crystals of FR-900109 p-bromophenyl ester were obtained from ethyl acetate. The crystal data of this compound are: C_{33}H_{36}O_{9}Br, monoclinic, a=15.732 (2), b=8.936 (1), c=11.245 (2) Å, β=106.6°, space group P2₁, D_{calc.} =1.44 g/cm³ and Z=2.

Intensity data were collected on a Rigaku automated four-circle diffractometer with graphite monochromated Cu-Kα radiation and 2160 independent reflections were used for the structure determination.

The structure was solved by the heavy atom method. Least-squares refinement with anisotropic temperature factors for all the atoms (except hydrogen) converged the conventional R factor to 0.065.

The stereochemistry of the molecule together with its molecular structure is shown in Fig. 1. The bond distances and angles within the molecule are presented in Figs. 2 and 3, respectively.

There are four rings in the FR-900109 molecule of which the main framework is composed of three rings, A, B and C. The five membered ring D is just attached to C(18) of ring C. The six membered ring A adopts a chair form but the form of ring B is slightly distorted owing to the double bond between C(14) and C(15). Ring C consists of six atoms, C(16), C(17), C(18), O(3), C(19) and C(20), and adopts a boat form of which the prows, C(18) and C(20), are bridged by oxygen atom, O(4). This complex ring can also be regarded to consist of a dioxolane ring, C(18)–O(3)–C(19)–C(20)–O(4), which is attached to ring B through bonds, C(16)–C(20) and C(17)–C(18).

The elongation of bond length such as C(16)–C(17) (1.60 Å) and the acute angle such as C(16)–C(17)–C(18) (95.8°) seem to be caused by a tension in this complex ring system.

Fig. 1. The molecular structure of FR-900109 p-bromophenyl ester.
The planar five membered ring D is attached to C(18). A rather high absorption frequency, 1830 cm\(^{-1}\) due to C=O stretching vibration in the infrared absorption spectrum\(^{1}\) is to be attributed to the strain in this ring D.

There are no short contacts less than 3.4 Å between the molecules in the crystal, which suggests no strong interaction between the molecules.

Reference