STUDIES ON A NEW ANTIBIOTIC FR-900109

2. X-RAY STRUCTURE DETERMINATION OF FR-900109 *p*-BROMOPHENYL ESTER

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(Received for publication February 24, 1983)

A new antibiotic called FR-900109 was obtained from streptomyces identified as *Streptomyces prunicolor* and its producing strain, fermentation, isolation procedures, chemical and biological properties have been reported in a previous paper[1]. 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: $C_{33}H_{35}O_9Br$, monoclinic, $a=15.732$ (2), $b=8.936$ (1), $c=11.245$ (2) Å, $\beta=106.6°$, space group $P2_1$, $D_{calcd.}=1.44$ g/cm^3 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.

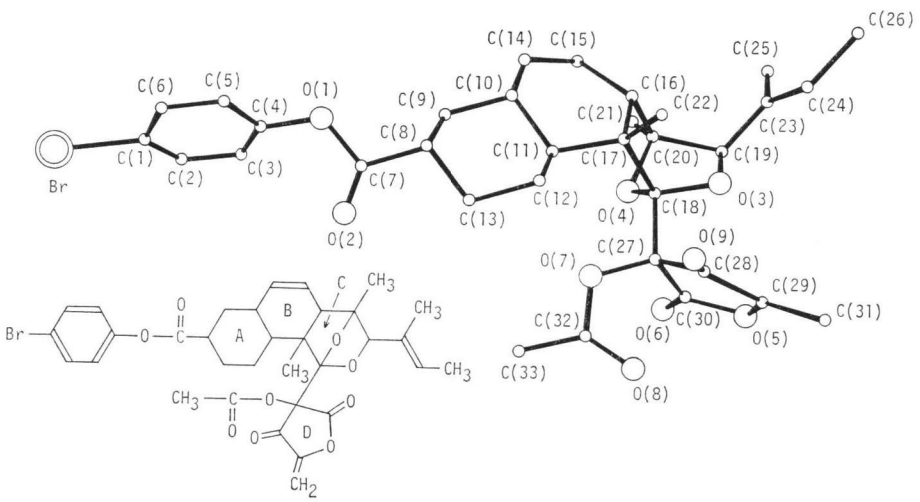


Fig. 2. Bond length (Å) in FR-900109.

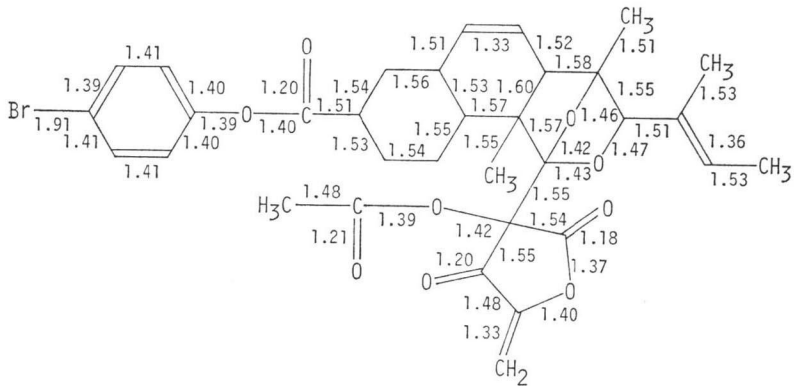
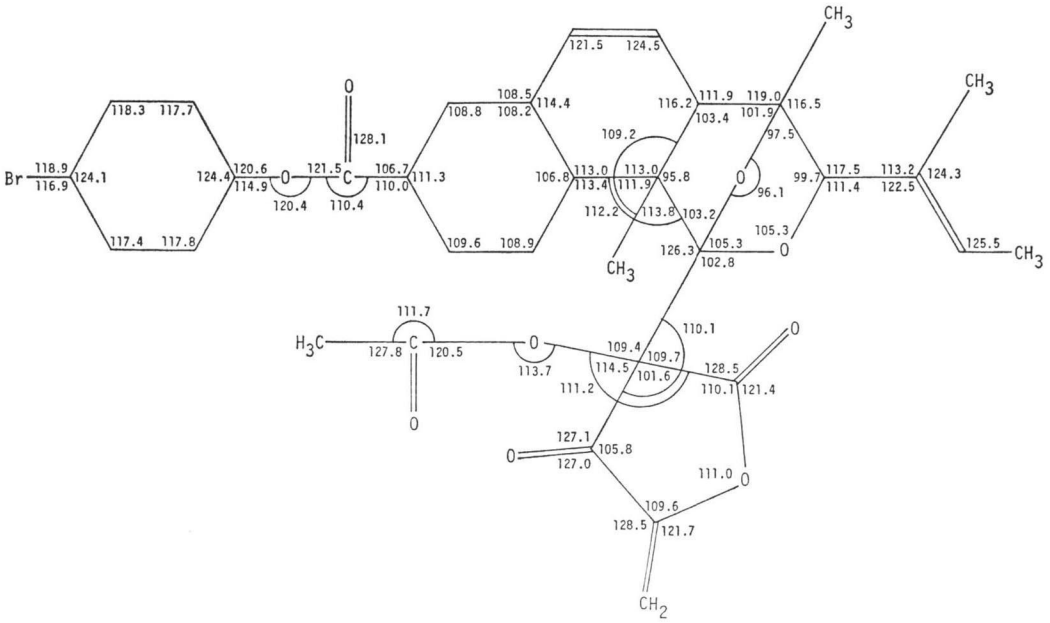


Fig. 3. Bond angles (°) in FR-900109.



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

1) YAMASHITA, M.; M. IWAMI, K. IKUSHIMA, T. KOMORI, H. AOKI & H. IMANAKA: Studies on a new antibiotic FR-900109. 1. Toxonomy, isolation and characterization. J. Antibiotics 36: 1123~1128, 1983