THE REVISED STRUCTURE OF ALBORIXIN

Sir:

In the polyether antibiotic family comprising more than forty members¹⁾, alborixin²⁾ and X-206³⁾ are characterized as having six cyclic ether systems, three hemiketal carbons and no methoxy substituent. The structures **I** and **II** in Fig. 1 both determined by X-ray analysis have been reported for alborixin²⁾ and X-206³⁾, respectively; the differences being the presence of a methyl function at C₆ in alborixin and the configuration at C₂₂*.

In an attempt to make complete assignments of the ¹³C-nmr spectra of these antibiotics, we compared the ¹³C-nmr spectral data of both the antibiotics measured in CDCl₃ solution at 25.05 MHz (TMS as internal standard). Taking account of the structural differences, the close similarities between the two spectra (Fig. 2) are more than expected. In particular, the chemical shifts of three hemiketal carbon signals (δ_C : C₂₇: 108.41, C₁₅ or C₂₁: 97.86 and 99.57 ppm in

alborixin and C₂₇: 108.34, C₁₅ or C₂₁: 97.74 and 99.52 ppm in X-206) are completely identical within experimental errors.

Since it is well known that the chemical shift of a given carbon is affected by the stereochemical modification at an adjacent carbon⁴⁾, this result strongly implies that the configuration at C₂₂ must be identical in both the compounds. Re-examination of the X-ray analytical data of alborixin and X-206 revealed that the stereochemistry of C₂₂ of the former must be amended so as to be identical with that of the latter.

Thus, the correct structure of alborixin is represented by **III** in Fig. 1. The error was caused by simple notational mistake in translating the three dimensional structure to the planar one²⁾.

HARUO SETO
KAZUTOSHI MIZOUE
NOBORU ÔTAKE

Institute of Applied Microbiology,
The University of Tokyo,
Yayoi, Bunkyo-ku, Tokyo,
Japan 113

Fig. 1. The structures of alborixin and X-206.

Fig. 2. ¹³C-NMR spectra of X-206 (**II**) and alborixin (**III**) free acids taken in CDCl₃ at 25.05 MHz. Chemical shifts are expressed in ppm from internal TMS. The signals for carboxylic acid [C₁: 176.21 in **II** and 176.41 in **III**] are not shown in this figure.

* The configuration at C₂₂ of X-206 was incorrectly represented in ref. 2.

PIERRE GACHON

ALAIN KERGOMARD

F.R.A. 10 INSERM and Laboratoire
de Chimie Organique Biologique,
Université de Clermont-Ferrand
B.P. 38, 63001 Clermont-Ferrand,
Cédex, France

JOHN W. WESTLEY

Chemical Research Department,
Hoffmann-La Roche Inc.
Nutley, New Jersey 07110, U.S.A.

(Received June 19, 1979)

References

- 1) WESTLEY, J. W.: "Polyether antibiotics: Versatile carboxylic acid ionophores produced by *Streptomyces*." in Adv. Appl. Microbiol. Vol. 22, pp. 177~223. Edited by D. PERLMAN, Academic Press, New York, 1977
- 2) GACHON, P.; C. FARGES & A. KERGOMARD: Alborixin, a new antibiotic ionophore: Isolation, structure, physical and chemical properties. J. Antibiotics 29: 603~610, 1976
- 3) BLOUNT, J. F. & J. W. WESTLEY: Crystal and molecular structure of the free acid form of antibiotic X-206 hydrate. J. Chem. Soc., Chem. Comm. 1975: 533, 1975.
- 4) STOTHERS, J. B.: "Carbon-13 NMR Spectroscopy". Academic Press, New York, 1972; LEVY, G. C. & G. L. NELSON: "Carbon-13 nuclear magnetic resonance for organic chemists". Wiley-Interscience, New York, 1972