Isopyrrolnitrin: A Metabolite from Pseudomonas

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Pyrrolnitrin (I) was isolated as a metabolite of Pseudomonas and its structure established by Arima and others.[1] During our investigation of metabolites of Pseudomonas, an isomer of pyrrolnitrin was found in the acetone extracts of the bacterial cells. First the existence of isopyrrolnitrin has been recognized by silica-gel thin-layer chromatography: R_f-values, 0.50 for pyrrolnitrin and 0.67 for isopyrrolnitrin, as determined by chloroform developing.

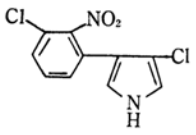
Isopyrrolnitrin has been isolated as yellowish crystals; m. p. 105—108°C, mol. wt. 257 by mass spectrometry.

Found: C, 46.82; H, 2.12; N, 11.27. Calcd. for $C_{10}H_6N_2O_2Cl_2$: C, 46.71; H, 2.35; N, 10.90%.

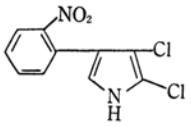
The infrared spectrum shows the presence of a –NH-group (3460 cm^{-1}) and characteristic absorption bands of the nitro group (1515 and 1349 cm^{-1}); the whole pattern of the spectrum is very similar to that of pyrrolnitrin. A color reaction by the Ehrlich reagent is positive (blue-violet). These data have suggested that isopyrrolnitrin has a structure similar to that of pyrrolnitrin. Conclusive information has been obtained from the NMR spectrum; the α-proton of the pyrrole ring appears at 6.76 p.p.m. as a doublet signal (coupling with the NH-proton of pyrrole), a proton adjacent to the nitro group in the benzen ring appears at 7.90 p.p.m. as a quartet signal, the multiplet signals from three protons appear at 7.3—7.7 p.p.m. of the aromatic proton region, and the proton of the NH-group appears at 8.4 p.p.m. as a broad signal (measured in $CDCl_3$ at 60 M c.p.s.). It follows from these data that the structure of isopyrrolnitrin is *o*-nitrophenyl-dichloropyrrole. The infrared absorption band at 743 cm^{-1} also shows that the compound is of a *o*-nitrophenyl substitution type, and the bands appearing in the region of 700—900 cm^{-1} are of a characteristic absorption which is common in the spectra of 2-substituted derivatives of pyrrolnitrin.

As a result of these studies, it may be supposed that the structure of isopyrrolnitrin is 2, 3-dichloro-4-(2′-nitrophenyl)-pyrrole (II). The correctness of this deduction has been proved by the synthesis.

The details will be published later.



(I)



(II)

1) K. Arima, H. Imanaka, M. Kousaka, A. Fukuta and G. Tamura, *Agr. Biol. Chem.*, **28**, 575 (1964).