X-Ray Crystal Structure of P-1894 B, a Collagen Proline Hydroxylase Inhibitor Produced by *Streptomyces albogriseolus* subsp. No. 1894

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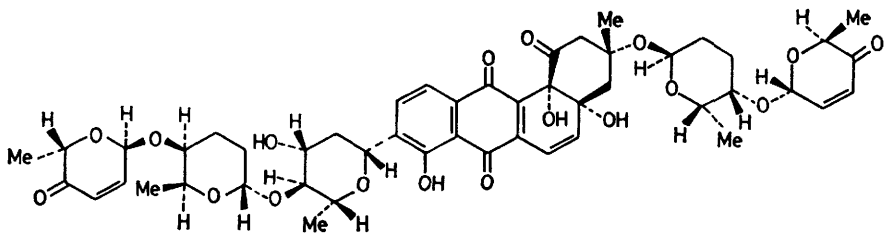
Summary The structure of P-1894 B, a collagen proline hydroxylase inhibitor isolated from the culture broth of *Streptomyces albogriseolus*, has been determined on the basis of physicochemical data and *X*-ray crystallographic analysis.

A POTENT collagen proline hydroxylase inhibitor, named as P-1894 B (**1**), was isolated from the culture filtrate of *Streptomyces albogriseolus* subsp. No. 1894.[1] The molecular formula of (**1**) ($C_{49}H_{58}O_{18}$) was estimated using microanalysis, vapour pressure osmometry, and ^{13}C n.m.r. spectrometry. The u.v., i.r., and ^{13}C n.m.r. spectra of (**1**), and its colour



(1)

reaction show that it has anthracycline chromophore and sugar groups. For a complete structural analysis, a single crystal *X*-ray analysis was carried out using a yellow needle of (**1**) recrystallized from a mixture of toluene and methanol.

Crystal data: Monoclinic, space group $P2_1$, $a = 27{\cdot}803(8)$, $b = 8{\cdot}078(3)$, $c = 13{\cdot}824(5)$ Å, $\beta = 92{\cdot}17(3)°$, $U = 3102(2)$ Å^3. Using monochromated Mo–K_α radiation (λ 0·71069 Å), 4400 independent reflections up to $2\theta = 45°$ were measured with a Rigaku AFC-5 diffractometer. A total of 3508 reflections with $F \geqslant 3\sigma(F)$ were used for the calculation of the structure. Based on the partial structure derived by direct methods with the program MULTAN,[2] the positions of the remaining non-hydrogen atoms in the molecule were found by successive electron-density syntheses. Hydrogen atoms and solvents of crystallization were located from difference electron-density syntheses. The structure was refined by the least-squares method with the program XRAY[3] and the *R* factor, at the present stage, is 0·078.† A perspective view of the molecule is shown in the Figure.

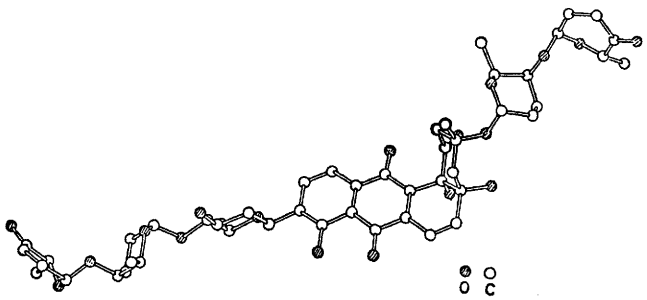


FIGURE.

Thus the structure of (**1**) was elucidated, but not its absolute configuration; this is the first example of a collagen proline hydroxylase inhibitor containing the benz[*a*]-anthracene structure.

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† The atomic co-ordinates for this work are available on request from the Director of the Cambridge Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW. Any request should be accompanied by the full literature citation for this communication.

[1] T. Ishimaru, K. Ohta, T. Kanamaru, and H. Okazaki, Abstracts Papers of 54th Annual Meeting of Agricultural Chemical Society of Japan, Tokyo, 1979, April 4, p. 373.

[2] P. Main, L. Lessinger, M. M. Woolfson, G. Germain, and J. P. Declercq, 'Multan 78, A Program for the Automatic Solution of Crystal Structures from X-ray Diffraction Data,' University of York, 1978.

[3] J. M. Stewart, P. A. Machin, C. Dickinson, H. Ammon, H. Heck, and H. Flack, 'The XRAY System, Version of 1976,' Tech. Rep. TR-446, Computer Science Center, Univ. of Maryland, College Park, Maryland.