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STRUCTURE OF VERSIOL, A NEW METABOLITE FROM *ASPERGILLUS VERSICOLOR*

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In the course of a continuing search for new metabolites of the genus *Aspergillus*,[1] we have isolated a new metabolite, named versiol, from a strain of *Aspergillus versicolor* (Vuillemin) Tiraboschi NI 5346. In this paper, we wish to report on the stereostructure of versiol determined by the X-ray diffraction method.

This mold was cultivated on malt extract medium. The chloroform extracts from the culture filtrate were chromatographed over silica gel and the elution with chloroform gave versiol. The compound, $C_{16}H_{22}O_3$, was crystallized from acetone to give colorless prisms, mp 180°C, $[\alpha]_D$-102° (c=1.5, $CHCl_3$). IR($CHCl_3$): 3600, 1700, 1640, 1610. NMR($CDCl_3$, 100 MHz): δ 1.04 (3H, d, J=7 Hz), 1.10 (3H, s), 1.27 (3H, s), 1.3 (1H, m), 1.95 (1H, exchangable), 1.95 (1H, m, J=14, 6, 4, 1.5 Hz), 2.35 (1H, m, J=15, 3.5, 1.5 Hz), 2.63 (1H, m), 2.85 (1H, m, J=15, 11, 9.5 Hz), 3.31 (1H, m, J=3.5, 3.5, 2.5 Hz), 3.96 (1H, m, J=12, 11, 3.5 Hz), 4.0 (1H, m), 4.07 (1H, m, J=12, 9.5, 1.5 Hz), 5.42 (1H, m, J=10, 1, 0.5 Hz), 5.71 (1H, m, J=4, 2.5, 1.5, 0.5 Hz), 6.19 (1H, d, J=10 Hz).

The cell constants of this crystal were obtained from Bragg angles measured by Toshiba four-circle diffractometer. The crystal data were as follows: M=262.35, orthorhombic, $P2_12_12_1$, a=9.14, b=6.11, c=25.20 Å, V=1408 Å^3, Z=4, D_x=1.24 g/cm^3. The intensities of 1065 independent reflections up to $\sin\theta/\lambda$=0.53 were measured with Ni-filtered Cu$K\alpha$ radiation. The stationary-crystal stationary-counter method was used, with a counting time of 30 seconds. The background for each reflection was taken from plots of the background as a function of 2θ. The intensities were corrected only for the Lorentz and polarization factors.

The structure was solved using the MULTAN program,[2] and refined by a block-diagonal least-squares program. The atomic species and the bond types were assigned on the basis of

temperature factors and interatomic distances and angles. The R value at the present stage is 0.08. The stereoscopic view of the molecule is shown in Fig. 1.

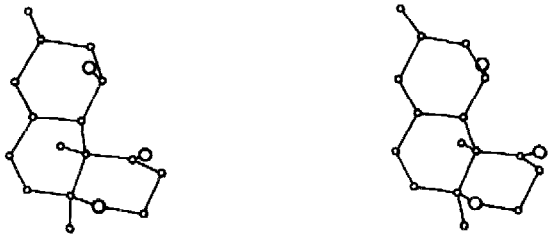
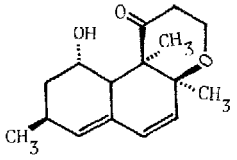


Fig. 1. The stereoscopic view of versiol. The small circles indicate carbon atoms, and large ones oxygen atoms. The hydrogen atoms are omitted for clarity, and no absolute configuration is implied.

From the present X-ray analysis, the structure of versiol is represented as 1. The distance between hydroxyl oxygen atom and carbonyl oxygen atom in a molecule is calculated to be 3.63 Å. Thus the chelation does not occur between the hydroxyl and carbonyl groups. However, there is an intermolecular hydrogen bond of O-H···O (2.90 Å). Recently, a metabolite, LL-N313β, whose structure is different from that of versiol in the stereostructure has been isolated from *Sporormia affinis* by McGahren *et al.*[3]



1

(This figure shows no absolute configuration.)

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