X-Ray Crystal and Molecular Structure of Acetylcolletotrichin (Colletotrichin), a Metabolite of *Colletotrichum capsici*

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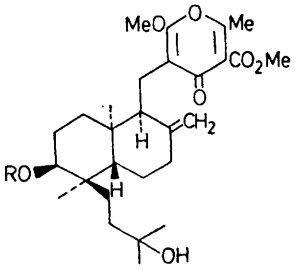
Summary From *X*-ray crystallographic data, the structure and relative stereochemistry is deduced for acetylcolletotrichin, a previously described metabolite of *Colletotrichum capsici;* since the metabolite does not contain an acetyl group, it is proposed that the name be changed to colletotrichin.

FROM the culture filtrates of the pathogenic fungus *Colletotrichum capsici*, Grove *et al.*[1] isolated a phytotoxic compound, $C_{28}H_{42}O_7$, which they named acetylcolletotrichin.



(1); R = H
(2); R = OAc

This metabolite has recently been shown[2] to inhibit mitochondrial respiration. We have now deduced the novel structure [(**1**) or enantiomer] for this fungal product from a single crystal diffraction study of the mono-acetate (**2**).

Since the metabolite (**1**) does not contain an acetyl group, it is suggested that the original[1] name be changed from acetylcolletotrichin to colletotrichin.

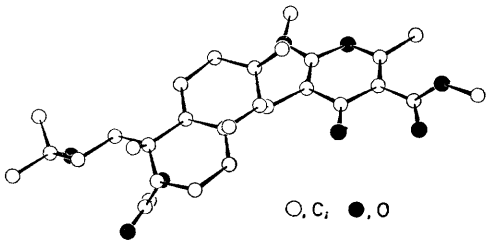


FIGURE. Molecular structure of the monoacetate of colletotrichin

Crystal data: $C_{30}H_{44}O_8$, M 532·63, orthorhombic, space group $P2_12_12_1$, a = 16·363(11), b = 11·921(3), c = 15·501(9) Å, Z = 4, D_c = 1·176 g cm^{-3}; Mo-K_α X-radiation (λ = 0·71069 Å), μ = 0·90 cm^{-1}. Data were collected on a Syntex $P2_1$, four-circle diffractometer (to 2θ = 50°). The structure (Figure) was solved by direct methods;[3] positional and anisotropic thermal parameters were refined by least squares. Of 3006 measured intensities, 1554 satisfied the criterion $I/\sigma(I) > 2·50$, and only these were used in the refinement of the structure;[4] R = 0·058.

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[1] J. F. Grove, R. N. Speake, and G. Ward, *J. Chem. Soc.* (*C*), 1966, 230.
[2] B. Foucher, J. B. Chappell, and J. D. McGivan, *Biochem. J.*, 1974, **138**, 415.
[3] G. Germain, P. Main, and M. M. Woolfson, *Acta Cryst.*, 1971, **A27**, 368.
[4] '*X*-Ray System of Programs,' Technical Report TR192 of the Computer Science Centre, University of Maryland, June 1972.