The Structure of a New Metabolite of *Aspergillus versicolor*

Sir:

In the previous communication¹⁾ we reported the structures of two pigments, versicolorin A and versicolorin B (I), which were isolated from mycelia of *Aspergillus versicolor* (Vuillemin) Tiraboschi. In addition to these compounds we subsequently isolated a new pigment, tentatively named versicolorin C, through chromatography on silica gel. In purifying the pigments we met difficulty which seems to have arisen from the close relation of their structures. This communication is concerned with the structure elucidation of versicolorin C.

Versicolorin C (II) is orange red needles, m.p. > 310°C, $[\alpha]_D^{25} 0^\circ$ (c. 0.44 in dioxane). *Anal.* Found: C, 63.55; H, 3.54; M.W., 332, 340 (osmometer). Calcd. for $C_{18}H_{12}O_7$: C, 63.53; H, 3.55%; M.W., 340. λ_{max}^{EtOH} 223(4.46), 255(4.20), 267(4.31), 292(4.46), 326(4.00), 450(4.03) m μ (log ϵ). ν_{max}^{KBr} 3410, 1670, 1625 cm⁻¹. Methylation of II gave a trimethyl ether (III), m.p. 216°C, $[\alpha]_D^{25} 0^\circ$, $[\alpha]_{590-600}^{25} 0^\circ$ (c 0.80 in dioxane). *Anal.* Found: C, 65.95; H, 4.87; OCH₃, 24.10; M.W., 386(osmometer), 380(Rast). Calcd. for $C_{21}H_{16}O_7$: C, 65.96; H, 4.75; OCH₃, 24.28%;

M.W., 382. λ_{max}^{EtOH} 223(4.58), 285(4.58), 346(3.52) 410(3.51) m μ (log ϵ). ν_{max}^{KBr} 1673, 1660 cm⁻¹. $\nu_{max}^{CHCl_3}$ 1665 cm⁻¹. The NMR spectrum of II in deuteriochloroform shows signals at 2.6 τ (singlet, 1 H); 2.69 τ (doublet, $J=2.5$ c.p.s., 1 H); 3.26 τ (doublet, $J=2.5$ c.p.s., 1 H); 3.63 τ (doublet, $J=6$ c.p.s., 1 H); 5.85 τ (multiplet, 2 H); 5.95 τ (singlet, 3 H); 6.02 τ (singlet, 3 H), 6.0 τ (singlet, 3 H); 6.35 τ (multiplet, 1 H), 7.7 τ (multiplet, 2 H).

The infrared spectrum of II showed a non chelated carbonyl band at 1670 cm⁻¹ and a chelated carbonyl band at 1625 cm⁻¹. The infrared spectrum of III showed a non-chelated carbonyl band at 1665 cm⁻¹ and no band due to the chelated carbonyl group. The ultraviolet spectrum of II was similar to that of versicolorin B, λ_{max}^{EtOH} 223(4.38), 255(4.13), 267(4.29) 291(4.38), 324(4.11), 450(3.94) m μ (log ϵ).¹ I, m.p. 298°C (decomp.), $[\alpha]_D^{25} -223^\circ$ (c 0.42 in dioxane), has the molecular formula $C_{18}H_{12}O_7$.¹

Similarity of the ultraviolet spectra of II to I, besides their same molecular formulas, suggests that both compounds would be very closely related hydroxyanthraquinone. How

FIG. 1. Infrared Spectra (in CHCl₃)

— Versicolorin B methyl ether
- - - Versicolorin C methyl ether.

1) T. Hamasaki, Y. Hatsuda, N. Terashima and M. Renbutsu, This Journal, **29**, 166 (1965).

ever, the difference can be seen in the melting points and optical properties. It is noticed that I is strongly levo-rotatory, whereas II is optically inactive.

The infrared spectra of II and I in Nujol showed close similarity except some slight differences. As both compounds are sparingly soluble in chloroform, the comparison of their infrared spectra was achieved using the solution of their methyl ethers, which gave superimposable spectra. The NMR spectrum of III in deuterochloroform gave a superimposable spectrum with that of methyl ether of I.¹⁾

Thus, the above experimental evidences in-

dicates that versicolorin C should be considered as a racemate of versicolorin B. As racemization of I was not observed in isolating procedure, II may be a natural product.

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