

The ^{13}C nmr spectrum of I showed an sp^3 carbon at 23.2 (C-2 Me). All the other carbons were sp^2 . There were signals for five fully substituted carbons at 103.9 (C-2), 110.3 (C-9) 117.9 (C-8), 119.3 (C-7) and 125.5 (C-3), two aromatic CH at 124.3 and 124.4 (C-5 and C-6), two OH-bearing carbons at 150.2 and 156.6 (C-4 and C-1) and a carbonyl at 195.8 (CHO). A signal at 119.6 was assigned to the exocyclic methylene.

The evidence presented here is compatible only with structure I. This structure may be looked at as an enolized form of a 2,3-dimethyl-1-indanone, stabilized by hydrogen bonding with the aldehyde carbonyl.

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Footnotes and References:

1. This culture was received from Dr. Ross W. Davidson (No. 24059), U.S.D.A., December 1943. Frustulosin was isolated in crystalline form and tested for biological activity in 1954.
2. The nmr spectra were taken in CDCl_3 solution with TMS as an internal standard, and are expressed in ppm values on the δ scale.
3. Applications of Nuclear Magnetic Resonance Spectroscopy in Organic Chemistry, 2nd edition, L.M. Jackman and S. Sternhell, Pergamon Press, New York (1969), p. 277.