CONSTITUENTS OF MOCHINEA POLYMORPHA

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As part of our continuing study of the genus *Mochinea* (Compositae) (1, 2), we are now reporting the isolation and identification of the sesquiterpene lactone dehydrocostus lactone (3) and a previously unknown, naturally occurring pentacyclic triterpene, bauerenyl acetate (1). This phyto-constituent was identical with bauerenol by comparison of the physical and chemical properties of its alkaline hydrolysis product. Subsequent Jones oxidation of our hydrolysis product furnished a ketone identical with bauerenone (4-6).

The cmr chemical shifts of compound 1 were assigned by comparison with models and on the basis of known substituent effects (7-11).

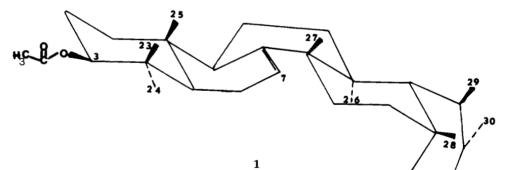
Previously unreported cmr data of **1** are described below.

This was characterized as dehydrocostus lactone (3).

Bauerenyl acetate.—Hexane extraction of the bark (500 g) furnished a precipitate (150 g), which after treatment with dry Et₂O and successive recrystallizations in CHCl₃-hexane (2:8), furnished a crystalline material (0.120 g), mp 290-292°, λ max (EtOH)=211 nm (ϵ =500);

$$\{\alpha\}\lambda^{24^{\circ}} = \frac{589}{-1.1 - 1.3 - 1.1 - 2.3 - 4.2^{\circ}} \operatorname{nm}(C=1.01)$$

 $\nu \max (\text{KBr}) 2857, 1730 (C=O, OAc) and 1235 cm⁻²; pmr (400 MHz, CDCl₃, TMS int. st.); <math>\delta$ 5.41 (d, H-7; J=2 Hz); 4.52 (dd, H-3, J=2; 2 Hz); 2.04 (s, -OCOCH₃); 1.06 (d, C-29 methyl, J=4 Hz) (12); 1.04 (s, C-27 methyl); 1.00 (s, C-26, methyl); 0.96 (s, C-24 methyl); 0.94 (s, C-23 methyl); 0.91 (d, C-30 methyl, J=2 Hz) (13); 0.85 (s, C-28 methyl) and 0.78 (s, C-25 methyl); ms showed peaks at m/z M⁺ 468 (25); 453 [M⁺-CH₃] (8); 392 (13); 288 (90); 228 [288-CH₃COOH] (68); 57 (88) and 43 (100%); cmr (63 MHz, CDCl₃, TMS standard, using PRFT and spin echo technique) (14, 15) ppm, C₁ 37.9,



EXPERIMENTAL

PLANT MATERIAL.—The trunk and bark of Mochinea polymorpha (Less.) DC. (3.0 kg) was collected in Campinas, São Paulo, Brazil, December 1979.

EXTRACTION AND ISOLATION.—The dry, powdered, plant material (trunk, 1.0 kg) was extracted with hexane to yield a yellow, gummy solid (8.0 g). The crude extract (6.0 g) was chromatographed on Si gel (120 g), and the CHCl₃ eluate gave a solid that partly crystallized. $C_2 24.1$, ${}^{1}C_3 81.3$, $C_4 36.8$, $C_5 50.8$, $C_6 24.3$, ${}^{1}C_7 116.5$, $C_8 145.6$, $C_9 55.3$, $C_{10} 35.3$, $C_{11} 29.4$, $C_{12} 29.7$, $C_{13} 32.2$, ${}^{1}C_{14} 41.4$, $C_{15} 17.0$, $C_{16} 32.7$, $C_{17} 31.7$, ${}^{1}C_{18} 48.7$, $C_{19} 35.6$, $C_{20} 38.0$, $C_{21} 29.1$, $C_{22} 37.9$, $C_{23} 15.5$, $C_{24} 27.6$, $C_{25} 13.1$, $C_{26} 22.7$, ${}^{1}C_{27} 22.5$, ${}^{1}C_{28} 25.7$, $C_{29} 23.7$, $C_{30} 21.1$, OCOCH₃-170,7 and OCOCH₃, 21.1. Compound **1** (30 mg) was hydrolized at 85°, for 6 h, in EtOH-KOH 5% solution and worked up in the usual way to give bauerenol (20 mg, mp 206-208°) (4).

¹May be interchanged.

Bauerenone.—Bauerenol (20 mg) was oxidized with Jones reagent at room temperature for 15 min to yield a ketone. Recrystallization of the ketone (12 mg) from CHCl₃ gave a product which showed ir and mass spectra identical with those described in the literature for bauerenone (4-6).

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LITERATURE CITED

- 1. T.C.B. Tomassini, B. Gilbert, *Phytochemistry*, **11**, 1177 (1972).
- M.E.O. Matos and T.C.B. Tomassini, *Phytochemistry*, **18**, 663 (1979).
- B.S. Mathur, S.V. Hiremath, G.H. Kulkarni, G.R. Kelber, and S.C. Bhattacharyya, *Tetrahedron*, 21, 3575 (1965).
- 4. F.N. Lahey and M.V. Leeding, Proc. Chem. Soc., 342 (1958).

- P. Serigupta and H.N. Khastgir, Tetrahedron, 19, 123 (1963).
- H. Budzikiewcz, C. Djerassi, D.H. Williams, "Structure Elucidation of Natural Products by Mass Spectrometry, Vol. II." San Francisco: Holden-Day, 1964, p. 131.
- E. Wenkert and B.L. Buckwalter, J. Am. Chem. Soc., 94, 4369 (1972).
- F.W. Wehrli and T. Wirthlin, "Interpretation of Carbon-13 NMR Spectra." London: Heyden, 1976, p. 64.
- 9. S. Seo, Y. Tomita, and K. Tori, Tetrahedron Lett., 7 (1975).
- H. Beierbeck and J.K. Saunders, Can. J. Chem., 53, 1307 (1975).
- A.G. Gonzalez, B.M. Fraga, O. Gonzalez, M.G. Hernandez, and A.C. Ravelo, *Phytochemistry*, **20**, 1919 (1981).
- T. Shingu, T. Yokoi, M. Niwa, and T. Kikuchi, *Chem. Pharm. Bull.*, **21**, 2253 (1963).
- S.K. Talapatra, S. Sengupta, and B. Talapatra, *Tetrahedron Lett.*, 5963 (1968).
- K. Nakanishi, V.P. Gullo, I. Miura, T.R. Gavindachi, and N. Viswanathan, J. Am. Chem. Soc., 95, 6473 (1973).
- 15. D.L. Rabenstein and T.T. Nakashima, *Anal. Chem.*, **51**, 1465 A (1979).

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