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LABIATAE

β-SITOSTEROL AND OTHER SUBSTANCES FROM *MONARDA CITRIODORA**

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Plant. Monarda citriodora. Gerv.

Source. Slopes of Chipinque, N.L., México.

Uses. Medicinal, diuretic and bacteriocide.

Previous work. The steam destillation provides an essential oil that contains more than 80% of thymol.[1] From the leaves of *M. didyma*, an isosakuranetin-7-β-rutinosid has been obtained.[2]

Present work. The aereal part (1540 g) was extracted successively with light petroleum, EtOH and H_2O. The petrol extract was saponified and the unsaponifiable part chromatographed on silica gel giving triacontane. $C_{30}H_{62}$ (m.p., mixed m.p., IR and NMR), and β-sitosterol $C_{29}H_{50}O$. (0·92 g, 0·26%) m.p., mixed m.p., $[\alpha]_D$ IR, NMR, and Co TLC of sterol, its acetate, its ketone). New compounds were also obtained. (*A*) $C_{29}H_{52}O_2$, m.p. 134–136°, $[\alpha]_D$ −238° ($CHCl_3$; c −0·5) ν_{max}^{KBr} 3440, 2920, 2860, 1640, 1450, 1380, 1368, 1050, 950, 880, 800 cm^{-1}. (Found: C, 80·04; H, 12·28; O, 7·39. Calc. for $C_{29}H_{52}O_2$; C, 80·49; H, 12·11; O, 7·40.) Liebermann–Burchard and tetranitromethane tests positives. Acetate, m.p. 115–117° $[\alpha]_D$ −34·4 ($CHCl_3$; c −1·0), ν_{max}^{KBr} 1725, 1640, 1450, 1240, 1040 cm^{-1}. (*B*) $C_{28}H_{52}O_2$, m.p. 62–63°, $[\alpha]_D$ −0·0° ν_{max}^{KBr} 2920, 2840, 1710, 1450, 1410, 1360, 730, 710 cm^{-1} no absorption in UV NMR δ^{CDCl_3}, 0·90 (m, 1·40 (s), 170 (m), 2·4–2·5 (m). (Found: C, 79·61; H, 12·28; O, 8·31.) The EtOH extract was chromatographed on silica gel, giving a third new compound. (*C*) $C_{19}H_{18}O_5$, m.p. 107–108°; $[\alpha]_D$ ±0·0; ν_{max}^{KBr} 3120 (wide), 3020, 2940, 2820, 2760, 2680, 1640, 1590, 1520, 1440, 1360, 1280, 1240, 1160, 960, 840, 765 cm^{-1}, λ_{max}^{EtOH} 204, (2218) 219 (2540) and 278 mm; (32,600) δ^{CDCl_3} 2·6 (s); 6·9 (d); (*J*, 9), 7·3 (n), 7·19 (d, *J*, 9). Acetate, oily, δ^{CDCl_3} 2·2 (s, 3H), 7·1 (d, *J*, 9) 7·6 (n). 7·8 (d, *J*, 9). (Found: C, 69·99; H, 5·70; O, 24·55. Calc. for $C_{19}H_{18}O_5$; C, 69·92; H, 5·56; O, 24·52%.)

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[1] R. W. SCORA, *J. Botany* **54**, 446 (1967).

[2] H. WAGNER, L. HORKAMMER, G. AURNHAMMER and L. FARKAS, *Chem. Ber.* **101**, 445 (1968).