CONSTITUENTS OF THE ESSENTIAL OIL OF *XANTHIUM CAVANILLESII*

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In a continuation of our research (1) on essential oils from Argentine indigenous plants, we now report the composition of an essential oil from *Xanthium cavanillesii* Schouw (Compositae). It is toxic to cattle; however, despite this fact, it is used as a leaf infusion in popular medicine (2). While some of the nonvolatile constituents of *X. cavanmillesii* (3) and other *Xanthium* species (4) are known, only the composition of the essential oil of *Xathium pennsylvanicum* (5) leaves has been reported for this genus.

The essential oil obtained by hydrodistillation of the aerial parts of the plant has the following physicochemical properties: yield 0.12% (W/W); $d^{20}{}_4=0.9324$; $n^{20}D=1.4859$; $[\alpha]^{20}D=+27.36°$; acid value 6.48; ester value 67.32.

Acidic compounds extractable with 5% aqueous $NaHCO_3$ represent 8.1% of the whole oil. Compounds identified were propionic, valeric, isovaleric, and salicylic acids. Phenolic compounds extractable with 7% aqueous NaOH represent 6.9% of the oil; isolated compounds were identified as thymol, carvacrol, *p*-cresol, pyrocatechol, and resorcinol. The resulting neutral essential oil was separated on silica gel into hydrocarbons (79.4% W/W) and oxygenated derivatives (20.6% W/W). The resulting fractions were studied by gc and gc/ms to aid in the identification of the components of the whole essential oil.

The gc of the whole oil indicated the following composition expressed as relative percents: α-pinene, 3.7; camphene, 2.4; β-pinene, 5.4; myrcene, 0.1; limonene, 43.6; *p*-cymene, 0.015; linalool, 0.8; α-thujone, 0.8; citronellal, 1.8; borneol, 3.6; α-terpineol, 1.1; carvone, 0.1; citronellol, 0.9; borynl acetate, 5.1; α-cubebene, 2.6; caryophyllene, 1.0; aromadendrene, 4.6; δ-cadinene, 3.1; nerolidol, 3.1; unidentified compounds 1.185%.

Monoterpene hydrocarbons (55.2%), especially limonene (43.6%), constitute the bulk of the essential oil; oxygenated monoterpenoids represent 14.2% and the sesquiterpene hydrocarbons 11.3%. A sesquiterpenic alcohol, nerolidol, is present in 3.1%, and only traces of the aromatic *p*-cymene were detected. As stated before, acids, represent 8.1%, phenols 6.9%, and several minor unidentified compounds 1.185%. The high limonene percent and the presence of α-pinene, comphene, myrcene, β-pinene, and borynl acetate are in agreement with the reported composition of *X. pennsylvanicum* essential oil (5).

EXPERIMENTAL

Green aerial parts of *X. cavanillesii* were collected at the beginning of the summer at Las Piedras, near Parana City (Entre Rios province, Argentina). Plant material was identified by J. Jozami, specimen voucher no. IPNAYS 127.

The oil was obtained by hydrodistillation (cohobation method) in a modified Clevenger apparatus for 11 h.

Analytical gc of the oil and fractions was conducted on a Hewlett Packard 5840 with FID detector without correction factors. Two columns were used: 10% Carbowax 20 M, 2.5 × 3.2 mm; and 10% OV 17, 2.5 m × 3.2 mm. For both columns oven temperature was programmed from 60° to 190° at 4° per min.

The gc/ms was performed by using the above gc columns and conditions combined with a Finnigan 4000 instrument. The acquired spectra matched with spectra stored in the NBS mass spectra library.

Phenols were isolated by preparative tlc on silica gel and identified by Rf and ir spectra against known compounds in the same conditions. Volatile free acids were identified in two ways: (*a*) by gc on Carbowax 20 M column, 150° isothermical; (*b*) an aliquot was carefully semi-microdistilled, and fractions controlled by gc. Ir spectra of pure compounds were registered as 0.25 mm film on a Perkin Elmer 180 spectrometer.

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