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CHEMISTRY OF SUDANESE FLORA:[1] *CYMBOPOGON NERVATUS*

B.M. MODAWI, H.R.Y. MAGAR, A.M. SATTI,

Chemistry Department, University of Khartoum, Khartoum, Sudan

and

R.J.H. DUPREY

Bush Boake Allen Ltd., Blackhorse Lane, London, E17 England

The genus *Cymbopogon* (Gramineae) contains 40 species, mostly native to the Old World Tropics, and constitutes an important proportion of savannah grass (1). Although taxonomic classification is often complicated by hybridization and polyploidy, probably nine species are found in Sudan (2,3).

The extracts of some of these species are widely used in folk medicine for the treatment of digestive ailments and as flavoring. A commercial preparation is claimed to show antispasmodic activity (4,5), to work as a diuretic (6), and to be an antihistaminic (7).

In a previous paper (8), the monoterpenes in the essential oil of *Cymbopogon nervatus* (Hochst.) Chiov. were isolated and completely characterized. The results revealed that the oil of this species falls into the 'menthane' class with the complete exclusion of acyclic and bicyclic monoterpenes. No attempts have been made to isolate the sesquiterpenoid components (about 5%) of the oil.

In our survey of the Sudanese flora chemistry (8,9), we report a comprehensive analysis of the essential oil from *C. nervatus* for its C-15 components and compare the results with those of *Cymbopogon proximus* previously characterized (8).

EXPERIMENTAL

PLANT MATERIAL.—Samples of foliage (*ca.* 500-100 g) from mature *C. nervatus* (Hochst.) Chiov. were collected from Abu Naama (Loam plain), Blue Nile Province, and identified by the Royal Botanic Garden, Kew, England. Specimens of the species were deposited in the herbarium of the Botany Department, University of Khartoum, Sudan.

EXTRACTION AND CHROMATOGRAPHY.—The steam-volatile oil was collected under N_2 using essentially the same procedures previously described in detail (10). The oil mixture (2.07% dry weight) was prefractionated using an efficient column to cut down the low-boiling point components.

The residual high-boiling-oil mixture, in C_6H_6, was carefully introduced on the top of a chromatographic column (87×2.5 cm) packed with silica gel (60-120 mesh). The sample was allowed to enter the column at a speed of 2 ml/min and eluted with C_6H_6/petroleum ether 40-60° (95:5) at the same speed. Fractions of 5 ml each were collected and monitored by tlc. All aliquots obtained were pooled into two samples and the solvent removed *in vacuo*.

The sample eluted last was subjected to further fractionation using a short column (43×2.5 cm) packed with silica gel (60-120 mesh) and C_6H_6-EtOAc (85:15) as eluent. Aliquots of 2 ml at a speed of 0.5 ml/min were collected and then resolved by tlc into three main components.

Individual constituents were further purified by preparative tlc using silica gel G/Kieselguhr (2:1 W/W) and petroleum ether 40-60° as eluent. Pure spots were carefully located with I_2 vapor, scraped off the plate, and extracted with Et_2O. The solvent was removed by flash distillation. Complete analysis and identification was conducted at the BBA (Bush Boake Allen Ltd.) For glc, the residual oil components were first prefractionated on SE-30 (3 m×0.5 cm), 10% W/W on Chromosorb G (80-100 mesh) programmed at 60-180° at 1.5 min^{-1} with N_2 flow rate of 3.6 liters h^{-1}. Each fraction was then chromatographed on Carbowax 20M (3 m×0.5 cm), 20% W/W on Celite (80-100 mesh) at 140° with flow rate of 3.1 liters h^{-1}.

Chemical identification was done by computer matching of the relative retention times from glc with data held at the memory bank and confirmed by comparing ^{1}H-nmr and ir spectra of column-tlc purified samples with those of authentic compounds.

[1]Part III in the series. For part I, see *Planta Med.*, **29**, 10 (1976) and for part II, see *Egypt. J. Chem.*, **22**, (5), 379 (1979).

RESULTS AND DISCUSSION

In part I (8), it was reported that the essential oil of *C. nervatus* contains about 5% unidentified sesquiterpene hydrocarbons. For the reinvestigation of the C-15 components in the oil of this species, it was essential to cut down carefully the low-boiling point compounds in order to accumulate a high proportion of sesquiterpenes in the residual oil mixture.

Comprehensive analyses of the residual oil led to the isolation and characterization of β-selinene, β-elemene, β-bergamotene, and germacrene-D, as the main components.

Both β-selinene and β-elemene were minor constituents (0.4% and 2%, respectively) in the sesquiterpenoid fraction of *C. proximus* essential oil (8), which contained mainly elemol (39%) and β-eudesmol (20%). Neither β-bergamotene nor germacrene-D was detected in the essential oil of *C. proximus* (8). Such a difference in oil composition was also observed in the monoterpenoid components of the genus *Cymbopogon*, inasmuch as 80% of the essential oil of *C. proximus* is piperitone, while the *p*-menthadienols constitute about 90% of the essential oil of *C. nervatus* (8).

The role of the germacrene nucleus as an intermediary in the biosynthesis of various sesquiterpene skeletal-types has been documented (11,12), and the working hypothesis is widely accepted (13,14).

The other interesting compound identified in the sesquiterpenoid fraction of the essential oil of *C. nervatus* is β-bergamotene, which was shown to be a key intermediate in the biosynthesis of ovalcinin produced by the fungus *Pseudoeurotum ovalis* (15-17). Such an antibiotic, antitumor, and immunosupressive compound has not been detected in the sesquiterpenoid fraction of the essential oil of *C. nervatus* nor in that of *C. proximus*. The only reference to such a physiologically-active principle was an uncharacterized sesquiterpene, $C_{15}H_{28}O_2$, mp 141-2°, $[\alpha]D$ −54.8 ($CHCl_3$), isolated from the essential oil of *C. proximus* (4) and claimed to have antispasmodic activity. Recently, Locksley *et al.* (18) have isolated an antispasmodic principle from the essential oil of *C. proximus* and identified it as cryptomeridiol, $C_{15}H_{25}O_2$, mp 141-142°, and $[\alpha]^{23}D$ −54.8 ($CHCl_3$). No such compound was detected in our sample.

Based on the fact that a number of species of the genus *Cymbopogon* are widely used in folk medicine, the presence of a bergamotene skeletal-structure as an intermediary suggests that this genus synthesizes such medicinally important compounds.

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