Journal of Chromatography, 262 (1983) 364–366
Elsevier Science Publishers B.V., Amsterdam — Printed in The Netherlands

CHROM. 15,765

Note

Composition of the essential oil of *Cymbopogon flexuosus*

JYRKI TASKINEN
Orion Pharmaceutical Laboratory, Espoo 10 (Finland)
and
D. K. MATHELA and C. S. MATHELA*
Chemistry Department, D.S.B.C. College, Kumaun University, Nainital-263002 (India)
(First received January 5th, 1983; revised manuscript received February 6th, 1983)

The genus *Cymbopogon* Spreng consists of about 85 species distributed in tropical and sub-tropical countries. A number of these species are aromatic and yield essential oils of commercial value. However, their identification has been a problem as they hybridize freely and also because some of them do not flower at all. Chemical taxonomy is of little help in this case, as morphologically indistinguishable grasses yield essential oils differing in composition and properties, while distinct species yield essential oils of almost identical composition (*e.g. C. citratus* and *C. flexuosus*).

Early studies showed that citral is the major component of the essential oil from *C. flexuosus* spp. However, more recent conventional and gas chromatographic (GC) investigations carried out by Atal and co-workers[1,2] led to the identification of geraniol and methyl eugenol as the major constituents of the essential oil of the RRL-57 chemotype of *C. flexuosus*, and of isointermedeol and further sesquiterpenoids in the RRL-4 type of this species. The present study is aimed at obtaining a detailed knowledge about the composition of the steam-volatile oil from common *C. flexuosus* (Steud.) Wats., cultivated in CIMAP farm, Nagla, India.

EXPERIMENTAL

Apparatus

A Carlo Erba, Model 2300, gas chromatograph coupled to a Jeol JMS-D300 mass spectrometer was used. The unit was attached to a JMA-2000 data system.

Materials and procedure

The essential oil was obtained by steam distilling the plant in a copper still, extracting the distillate with light petroleum (b.p. 60–80°C), drying (sodium sulphate) and concentrating the organic phase under reduced pressure (yield 0.6%).

The oil was analysed by GC–mass spectrometry (MS) using a glass capillary column (38 m × 0.3 mm I.D.) with FFAP as the stationary phase. The column temperature was maintained at 60°C for the first 6 min, then raised to 100°C and programmed at +4°C/min up to 200°C. The mass spectra measured at 70 eV were scanned automatically at intervals of 2.5 sec. The injection port, interface and ion source temperatures were 250, 220 and 230°C, respectively.

0021-9673/83/$03.00

Preseparation and GC–MS analysis of the hydrocarbon fraction

The oil (200 μl) was placed at the top of a column of silica gel (10 × 1 cm) and the hydrocarbons were eluted with 100 ml of *n*-pentane. After concentration in a vacuum evaporator, the eluate was analysed by GC–MS using a glass capillary column (50 m × 0.3 mm I.D.) with SP-2100 silicone polymer as the stationary phase. Conditions: sample, 0.3 μl (injection split ratio, 1:100); temperature programming from 80 to 200°C at +5°C/min; injection port, interface and ion source adjusted to 250, 220 and 230°C, respectively. The mass spectra (70 eV) were scanned repetitively from *m/z* 25 to 250 with a 1.5-sec cycle.

RESULTS AND DISCUSSION

The gas chromatograms of the oil and hydrocarbon fraction are shown in Figs. 1 and 2, respectively. The individual constituents were identified by comparing their mass spectra with those of authentic samples and with published mass spectral data[3–8].

In the chromatogram of the whole oil, the sesquiterpenes are overshadowed by oxygen-containing monoterpenes. This difficulty could be efficiently circumvented by preseparating the hydrocarbon fraction by silica gel chromatography. The GC–MS study of this hydrocarbon fraction led to the identification of seven mono- and eight sesquiterpene hydrocarbons.

The carbonyl compounds determined by the hydroxylamine method[9] constitute 65% of the oil, citral (neral and geranial) being the principal component (60%). Further constituents are geraniol (5%), hydrocarbons (8%), and trace amounts of methyl eugenol. These results sharply contrast with those reported for the essential oils of two chemotypes of *C. flexuosus*, whose major constituents were found to be sesquiterpene alcohols (56%; isointermedeol 50.56%) and hydrocarbons (21.2%) (in RRL-4 type[1]), and geraniol (40%) and methyl engenol (20%) (in RRL-57 type[2]).

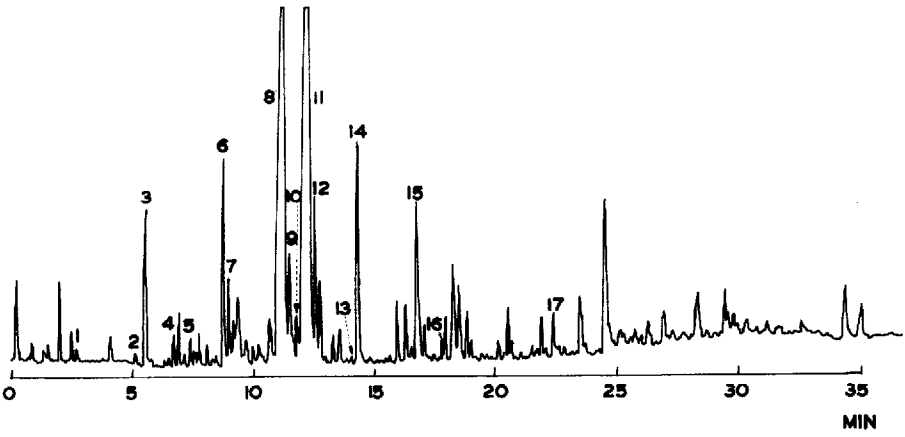

Fig. 1. Gas chromatogram of the essential oil of *Cymbopogon flexuosus* on a glass capillary column (38 m × 0.3 mm I.D.) coated with FFAP. For conditions, see text. The peaks numbered in the chromatogram are those of oxygen-containing terpenes. Peaks: 1 = 1,8-cineole; 2 = 3,7-dimethyl-7-octen-1-ol; 3 = 6-methyl-5-hepten-2-one; 4 = perillene; 5 = menthone; 6 = linalool; 7 = linalyl acetate; 8 = neral; 9 = neryl acetate; 10 = piperitone; 11 = geranial; 12 = nerol; 13 = *p*-cymen-8-ol; 14 = geraniol; 15 = sesquiterpene alcohol (mol.wt. 220); 16 = methyl eugenol; 17 = elemicin.

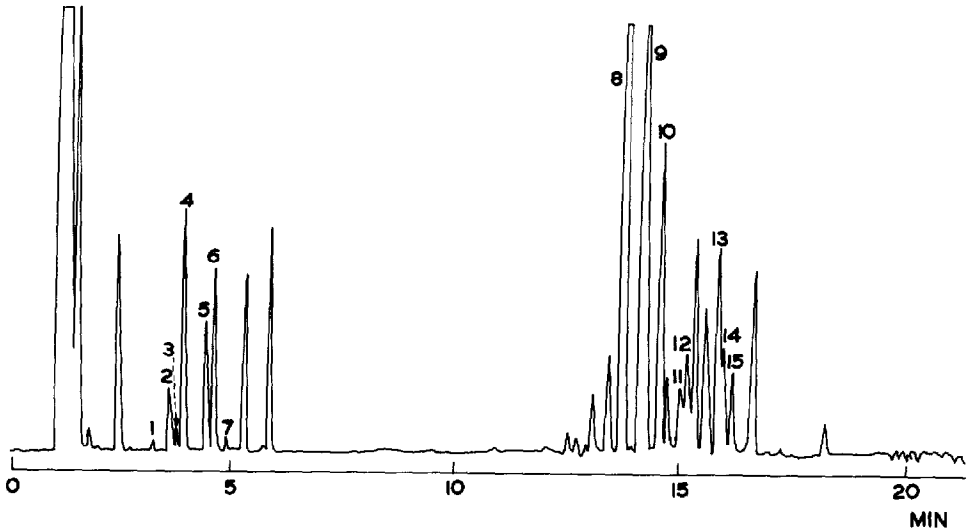

Fig. 2. Gas chromatogram of the hydrocarbon fraction of the oil on a glass capillary column (50 m × 0.3 mm I.D.) coated with SP-2100. For conditions, see text. Peaks: 1 = α-pinene; 2 = β-pinene; 3 = sabinene; 4 = myrcene; 5 = limonene; 6 = *p*-cymene; 7 = 3,7-dimethyl-1-octene; 8 = trans-caryophyllene; 9 = α-bergamotene; 10 = α-humulene; 11 = γ-muurolene; 12 = α-curcumene; 13 = β-bisabolene; 14 = γ-cadinene; 15 = δ-cadinene.

ACKNOWLEDGEMENTS

We are grateful to the authorities of M/s Orion Pharmaceutical Laboratory, Espoo, Finland, for GC–MS facilities and to Dr. S. P. S. Duhan, CIMAP, Nagla, India, for cultivating the plant.

REFERENCES

1 R. K. Thappa, K. L. Dhar and C. K. Atal, *Phytochemistry*, 18 (1979) 671.
2 C. K. Atal and B. L. Bradu, *Indian J. Pharm.*, 38 (1976) 63.
3 R. Ryhage and E. von Sydow, *Acta Chem. Scand.*, 17 (1963) 2025.
4 J. Andersson and E. von Sydow, *Acta Chem. Scand.*, 18 (1964) 1105.
5 Y. Masada, *Analysis of Essential Oils by Gas Chromatography and Mass Spectrometry*, Wiley, New York, 1976.
6 M. G. Moshonas and E. D. Lund, *Flavour Ind.*, 1 (1970) 375.
7 E. von Sydow, *Acta Chem. Scand.*, 19 (1965) 2083.
8 J. A. Gilpin and F. W. McLafferty, *Anal. Chem.*, 29 (1957) 990.
9 E. Guenther, *The Essential Oils*, Vol. 1, Van Nostrand, New York, 1949, p. 286.