Phytochemistry, Vol. 21, No. 3, p. 793, 1982.
Printed in Great Britain.

0031-9422/82/030793-01$03.00/0

ISOLATION AND IDENTIFICATION OF PHENOLS IN OIL OF VETIVER

TAKAYUKI SHIBAMOTO and OSAMU NISHIMURA*

Department of Environmental Toxicology, University of California, Davis, CA 95616, U.S.A.; *Ogawa & Co. Ltd., 6-32-9 Akabenenishi, Kita-Ku, Tokyo, Japan

(*Received* 1 *May* 1981)

Key Word Index—*Vetiveria zizamioides*; Gramineae; vetiver oil; phenols.

Abstract—Several rare phenols, including 4-vinylphenol, 4-vinyl-2-methoxyphenol and *trans*-isoeugenol, were identified in oil of vetiver.

INTRODUCTION

Oil of vetiver is obtained from the dried roots of *Vetiveria zizamioides* (Gramineae), a native of India, by steam distillation and has been widely used in cosmetics. The major components of the oil are sesquiterpenes. Approximately 60 constituents have so far been identified [1–4]. In this study, we report the occurrence of several phenol derivatives which have not so far been noted.

RESULTS AND DISCUSSION

The phenolic fraction of vetiver oil was isolated by successive extraction (see Experimental) and subjected to GC and both MS and NMR. Eleven compounds were identified including 4-vinylphenol, 4-vinyl-2-methoxyphenol, and *trans*-isoeugenol (Table 1). Such derivatives have been found in various essential oils. For example, *p*-cresol is present in ylang ylang and jasmin oils. Eugenol exists in clove, cinnamon and violet oils while guaiacol has been found in guaiac resin, orange leaves, tobacco leaves, and nutmeg oils [5]. Recently, some phenols were found in coffee beans [6, 7]. Such phenols have not been reported, however, in oil of vetiver prior to this study.

Zizanoic acid was found in the weak acidic fraction of vetiver oil in large quantity, comprising over 90% of the strong acidic fraction. It is known that the oil of vetiver contains many other interesting chemicals. The presence of large quantities of both acidic and possibly basic compounds makes GC analysis difficult without proper prior treatment and further study is necessary in order to identify the remaining acidic and basic constituents of the oil.

Table 1. Volatile compounds identified in the weak acidic fraction

Peak No.	Compound	Peak area (%)
1	Methoxyphenol	0.0048
2	*o*-Cresol	0.0076
3	*p*-Cresol	0.0062
4	*m*-Cresol	0.0045
5	Eugenol	0.0056
6	4-Vinylguiacol	0.154
7	*cis*-Isoeugenol	0.011
8	*trans*-Isoeugenol	0.132
9	4-Vinylphenol	0.421
10	Vanillin	0.0014
11	Zizanoic acid	3.25

EXPERIMENTAL

Oil of vetiver was obtained from dried roots of the plant by steam distillation and was dissolved in Et_2O (3 ml/g) and washed with 5% $NaHCO_3$ to remove strong acidic components. The Et_2O layer was subsequently washed with 2% NaOH soln and the aq. soln re-extracted with Et_2O. The pH of the aq. soln was then adjusted to 5–6 with 6NHCl and extracted with Et_2O to give the weak acidic fraction. This extract was washed with dil. NaCl and dried (Na_2SO_4). The solvent was evapd, yielding a brown oily liquid (1.56%). Identification of the oil constituents was based on GC/MS (Hitachi M-80) and confirmed by GC retention data (Kovats, 1958). Some major peaks which could not be identified by the above method were isolated by TLC (Merk Si gel 60, F-254; solvent, C_6H_6–$CHCl_3$ = 7 : 3) and prep. GLC (Hitachi M-5201 equipped with TCD, and 2 m × 4 mm glass column packed with 5% Carbowax 20M on 60/80 mesh Chromosorb W).

4-Vinylphenol was obtained by TLC (R_f = 0.19–0.30). The materials recovered from TLC at R_f = 0.38–0.56 were further separated by prep. GLC and were identified by NMR (Hitachi R-20 A) and IR (Hitachi EPI-G3) by comparing their spectra to those of authentic samples.

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