Headspace Constituents of Vetiver Oil

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By headspace analysis of the essential oil of Vetiver hitherto sixteen not described volatile constituents, mainly monoterpenes, could be identified. For these investigations GC-FID, GC-MS, GC-FTIR and the GC-sniffing-technique were used.

Introduction

The essential oil of Vetiver (Vetiver zizanoides Stapf.) is a valuable raw material in perfumery [1–6]. More than 150 constituents of Vetiver oil with eleven different sesquiterpene main structures were described [7–9]. The responsible compounds for the typical Vetiver odour still are unknown until today.

The aim of this investigation was the identification of the main volatile odour components in the headspace of Vetiver oil using GC-MS and GC-FTIR in combination with the GC-sniffing-technique and olfactoric evaluation to get more information about the composition of the precious woody odour of this root oil.

Results and Discussion

The headspace of the Vetiver oil was trapped by the use of a commercial pumping and trapping system and investigated by means of GC-FID, GC-MS and GC-FTIR. Thirteen known sesquiterpenic compounds as constituents of the essential oil of Vetiver [7, 9] could be identified herein (see Table I) and the structure of another sixteen, until now not described constituents were elucidated by correlation of their spectra with published data [7] or library spectra.

These new constituents are mainly monoterpenes (see Table II). Their spectral data were correlated also with their odour impression activity using the GC-sniffing-technique and olfactoric evaluation of the single compounds. The described "characteristic precious wood- and root-like, long lasting odour" [2] could not be associated to anyone of the new constituents by these odour experiments, but they appear to be important for the top note of this oil and may have valuable synergistic effects with the other "typical Vetiver odour compounds".

Table I. Identified sesquiterpene constituents in the headspace of Vetiver oil.

No.	Compound	Mwt
1	α-Calacorene	200
2	β-Vetivene	202
3	(−)-Selina-4(14),7(11)-diene	204
4	(−)-γ-Cadinene	204
5	Zizanene	204
6	Zizaene	204
7	Prezizaene	204
8	α-Cedrene	204
9	Alloaromadendrene	204
10	β-Vetivone	218
11	α-Vetivone	218
12	Khusimol	220
13	Isovalesenol	220

Table II. New constituents in the headspace of Vetiver oil.

No.	Compound	Mwt
1	2-Methyl-2-butenal	84
2	Furfural	96
3	*n*-Octane	114
4	2-Acetyl-5-methylfurane	124
5	2-Butylfurane	124
6	*p*-Cymol	134
7	α-Thujene	136
8	α-Pinene	136
9	β-Pinene	136
10	Camphene	136
11	Myrcene	136
12	Limonene	136
13	Carane	138
14	2-Pentylfurane	138
15	1,8-Cineole	154
16	1-Phenylethyl acetate	164

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Experimental

The essential oil of Vetiver (Bourbon, Reunion) was obtained from Dragoco Comp.

Headspace: Pumping and trapping system G 24/02 from H. Brey Comp. Germany with absorption charcoal tubes Lot 120 Niosh Approved from SKC Inc. USA. Trapping-time: 12 h and desorption with 150 μl of CS_2 or CH_2Cl_2.

GC: A HRGC-Mega-Series from the Carlo Erba Comp., 25 m HP-20 M fused silica capillary column (Carbowax 20 M, 0.2 mm i.d. and 0.2 μm film thickness) from Hewlett-Packard Comp. Temp.-prog.: 35 °C/2 min to 150 °C with a heating rate of 5 °C/min and than to 280 °C with a heating rate of 20 °C/min, injector: 250 °C, detector (FID): 300 °C, carrier gas: hydrogen, split ratio: 1:20.

GC-MS: Varian 3400 gas chromatograph with Finnigan MAT INCOS 50 mass spectrometer and DATA GENERAL MicroECLIPSE data system; 70 eV, scan time: 0.73 sec., mass range: 40–300 amu, carrier gas: helium, ion source: 160 °C, interface: 280 °C; other parameters see GC part.

GC-FTIR: A HP-5890 A GC with HP-5965 B IRD (MCT detector) and data system HP-59970 C ChemStation, range of 4000 to 800 cm^{-1}; Other parameters see GC-MS part.

Spectral library search: MS spectra were correlated with NBS and Wiley (on line) or NIST and FOOD (off line) and the IR spectra with EPA and ROBERTET (on line) library.

GC-Sniffing-technique: Fractovap-2101 GC with LT-Programmer-230 and Electrometer-160 (Carlo Erba Comp.), printer: Kompensograph III (Siemens Comp.); Carrier gas: hydrogen, split: 1:50 = FID/nose, column: 30 m HP-FFAP mega bore fused silica (Hewlett-Packard, 0.53 mm i.d. and 1.0 μm film thickness), injector: 250 °C, detector (FID): 260 °C, sniffing capillary heating: 250 °C; Other parameters see GC part.

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