Journal of Pharmacognosy and Phytochemistry
Available online at www.phytojournal.com

E-ISSN: 2278-4136
P-ISSN: 2349-8234
JPP 2018; 7(6): 1709-1713
Received: 28-09-2018
Accepted: 30-10-2018

M Bharathi Raja
Department of Medicinal and Aromatic Crops, Horticultural College and Research Institute, Tamil Nadu Agricultural University, Coimbatore, Tamil Nadu, India

K Rajamani
Department of Medicinal and Aromatic Crops, Horticultural College and Research Institute, Tamil Nadu Agricultural University, Coimbatore, Tamil Nadu, India

J Suresh
Department of Spices and Plantation Crops, Horticultural College and Research Institute, Tamil Nadu Agricultural University, Coimbatore, Tamil Nadu, India

A John Joel
Department of Plant Genetic Resources, Tamil Nadu Agricultural University, Coimbatore, Tamil Nadu, India

D Uma
Department of Biochemistry, Tamil Nadu Agricultural University, Coimbatore, Tamil Nadu, India

Correspondence
M Bharathi Raja
Department of Medicinal and Aromatic Crops, Horticultural College and Research Institute, Tamil Nadu Agricultural University, Coimbatore, Tamil Nadu, India

Chemical composition of Vetiver root oil obtained by using GCMS analysis

M Bharathi Raja, K Rajamani, J Suresh, A John Joel and D Uma

Abstract
Essential oil from roots of *Chrysopogon zizanioides* (L.) Roberty, analyse were performed using by gas chromatography mass spectrometry (GC/MS), and about 32 compounds were identified in root oil, mainly sesquiterpenes. The characteristic constituents were Valerenol (19.88%), beta-Vatirenene (8.61%), Longiverbenone (3.46%), Germacrene D (3.82%), Aristolene (3.20%), Selin-6-en-4-o (2.99%) and Globulol (2.18).

Keywords: *Chrysopogon zizanioides*, vetiver essential oil, chemical composition, GC/MS

Introduction
Vetiveria zizanioides (L.) Nash (syn. *Chrysopogon zizanioides* (L.) Roberty) is a perennial grass, rhizomatous, with culms up to 2m height. This species is native of India and has been introduced in many tropical countries (Java, Haiti, Reunion, *etc*.). The plant is grown for its aromatic roots, source of essential oil known as oil of vetiver. This oil is principally used in high class perfumery where its persistent odour makes its great value as a fixative and perfumery. Indonesia, China and Haiti are major producers. About 60 to 75 tons of vetiver oil are annually produced from Indonesia and Indonesia becomes the major supplier of vetiver oil in the world (Putrawan *et al*., 2015) [14]. The annual world trade in vetiver oil is estimated around 250 tons with Haiti, Indonesia, China, Japan, India and Brazil being the main producers and USA, Europe, India and Japan being main consumers, (Dalton *et al*., 1996) [6].

Vetiver oil is traditionally known as vetiver oil in trade. It is also known as "oil of tranquality" and has a distinct fragrance with no synthetic substitute available (Chahal *et al*., 2015) [2]. Vetiver is one of the most important raw materials in perfumery both as a fixative and in its own right as fragrance ingredient (Lavania, 2003) [10]. Recent research has found new biological activities of vetiver oil and its components such as antifungal, antibacterial, anticancer, anti-inflammatory and antioxidant activities (Kim *et al*., 2005) [8].

Vetiver oil is obtained from roots of vetiver grass by steam distillation and hydrodistillation. Extraction of vetiver oil from grass is known in India since time of vedas. It is viscous, light to dark brown oil obtained from aromatic roots by stem distillation methods. Depending upon the biotype, cultural practices, age of root, mode and duration of distillation vetiver may yield about 0.3 to 2 % essential oil on fresh root weight basis, (Lal *et al*., 1998).

Vetiver oil extracted from North Indian variety has the typical earthy note, higher specific gravity, free alcohols and ester value after acetylation while the South Indian has the dominant spicy character, higher refractive index, acid value and ester value. More than 150 constituents have been identified in vetiver root oils produced in different countries, (Chowdhury, 2002) [8]. Now a days, approximately 3000 essential oils are known of which 300 are commercially available. The major constituents of essential oils are terpenes/terpenoids, aromatic and aliphatic compounds, which are characterized as low-molecular weight aroma chemicals responsible for various properties of the plant. The present investigation was undertaken to determine the chemical composition of root oil of *V. zizanioides*.

Material and methods
Planting materials
The plant material of vetiver roots (14 month old) was collected from the Botanical garden, Department of Medicinal and Aromatic crops, Tamil Nadu Agricultural University, Coimbatore, Tamil Nadu, India. Samples of root were harvested from healthy, well-grown plants, cleaned and air dried for 5 days in the shade.

Extraction of oil

The air dried roots (100 g) were powdered and subjected to hydrodistillation in a Clevenger glass apparatus for 10 hours for isolation of oils, followed by removal of the solvent by evaporation over a steam bath. Yield was calculated using the following equation:

$$\text{Essential oil content (\%)} = \frac{\text{Quantity of essential oil collected}}{\text{weight of roots (100 g)}} \text{ x } 100$$

Gas Chromatography-Mass Spectrometry

The GC/MS analysis of essential oil of vetiver [*Chrysopogon zizanioides* (L.) Roberty] was performed using Thermo Trace Ultra GC system equipped with Tri Plus RSH auto sampler DSQ mass selective detector (Thermo Scientific Co.,). Compounds were separated on ZB-35 MS capillary column having 35 per cent phenyl polysiloxane as stationary phase, column length 30.0 m, internal diameter 0.25 mm and film thickness 0.25 um. The temperature of injector was 2500 C and 1.0 uL of sample was injected in the split less mode. Helium (He) was used as carrier gas, and the flow rate of gas was 1.0 Ml min-1. The temperature program was: initial temperature 70 °C and held for 1 min, then ramping at a rate of 6°C / min up to 260°C and finally held at this temperature for 10 min. The temperature of MSD transfer line was 280°C. For mass spectra determination, MSD was operated in electron ionization (EI) mode, with the ionization energy of -70 eV, while the mass range scanned was 50-650 m/z. The temperature of ion source was 220°C. The identification of components was based on comparison of the obtained mass spectra with those of NIST Ver: 11 and WILEY mass spectral library. The GC/MS analysis of the oil sample distilled from root yield enabled the identification of aroma components. The mass spectrum of each compound was compared with the NIST 11 library. Library data of the peaks with those reported in literature, mass spectra of the peaks with literature data. Percentage composition was computed from GC peak areas on BD-5 column without applying correction factors.

Result and discussion

Analysis and identification of chemical composition of vetiver oil were most widely used gas chromatography/mass spectrometry (GC/MS). The chromatograms GC of vetiver oil are shown in Fig. 1, whereas the chemical compositions of vetiver oil are shown in Table 1. Thirty two compounds were identified oils. The presence of chemical compounds *viz*., revealed the presence of Beta-Vatirenene, Valerenol, Ariston's, Germacrene D, Alloaromadendrene, alfa-Copaene, Longiverbenone, Alpha –Ylangene, Alpha – Amorphene, Selin-6-en-4-o, Globulol, Alpha–Longipinene, bete - Copaene, Gamma-himachalene, Nootkatone and Alpha – Gurjunene, which have various bioactivities. Among them, the highest area percentage was recorded in Valerenol (19.88 %) followed by beta-Vatirenene (8.61%), Longiverbenone (3.46%), Germacrene D (3.82%), Aristolene (3.20%), Selin-6-en-4-o (2.99%) and Globulol (2.18%). (Champagnat *et al*., 2006 [3]; Chahal *et al*., 2015 [2]; Kadarohman *et al*., 2014 [7]; Yanto *et al*., 2016 [15]; Bhuiyan *et al*., 2008 [1]; Chou *et al*., 2012 [4]; Kim *et al*., 2005 [8]; Martinez *et al*., (2004); Pripdeevech *et al*., (2006) [13] and Mallavarapu *et al*., (2012) [11], reported occurrence of similar constituents in essential oil of vetiver).

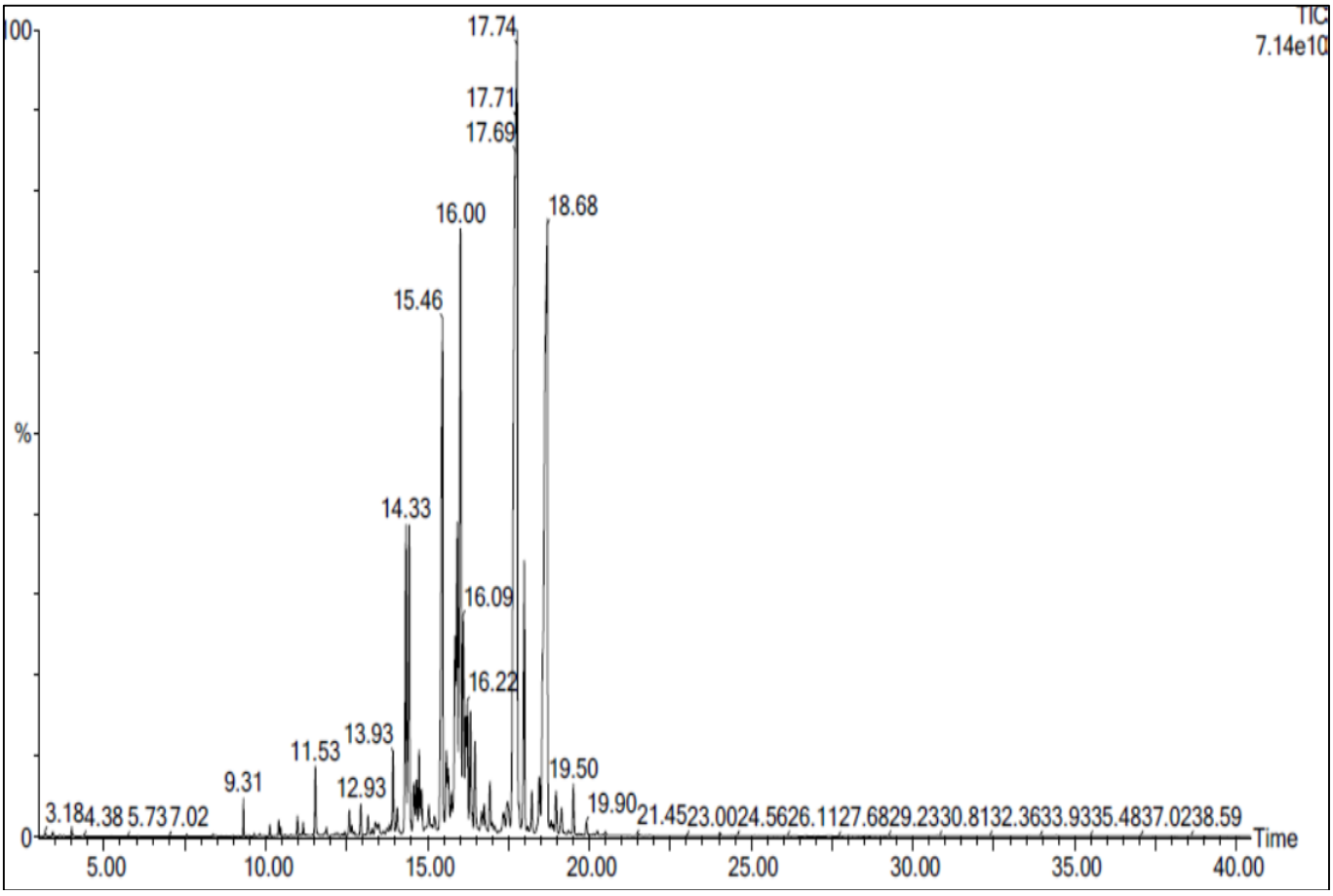
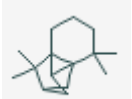
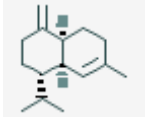
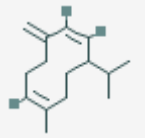
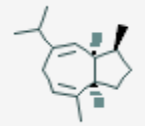
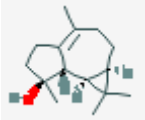
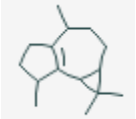
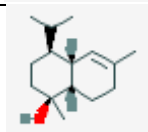
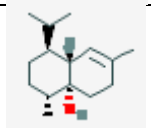
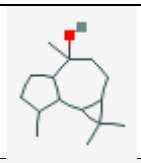
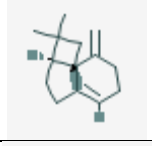
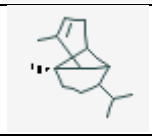
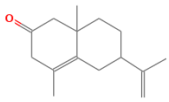
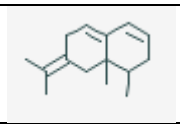
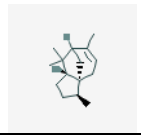
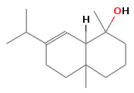
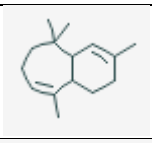
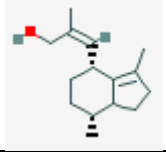
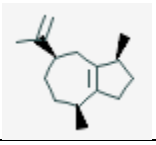
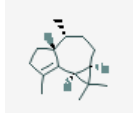
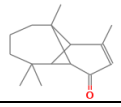
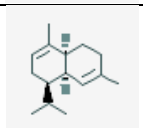
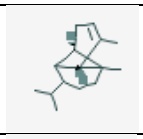
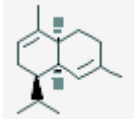
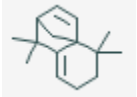


Fig 1: Chromatogram GC of vetiver oil

Table 1: Chemical composition of vetiver oil by GC/MS analysis

S. No.	Name of the compound	Molecular Formula	Molecular weight	Structure	Peak area (%)
1.	Cycloisolongifolene	$C_{15}H_{24}$	204.357 g/mol		0.20
2.	All-oaromadendrene	$C_{15}H_{24}$	204.357 g/mol		0.77
3.	Alpha –copaene	$C_{15}H_{24}$	204.357 g/mol		0.28
4.	gamma-Muurolene	$C_{15}H_{24}$	*mol/g 204.357*		0.35
5.	Germacrene D	$\boldsymbol{C}_{15}H_{24}$	204.357 g/mol		3.82
6.	Guaia-6,9-diene	$C_{15}H_{24}$	204.357 g/mol		0.77
7.	Isolongifolol	$C_{15}H_{26}O$	222.372 g/mol		0.14
8.	Isospathulenol	$C_{15}H_{24}O$	220.356 g/mol		0.45
9.	Isoledene	$C_{15}H_{24}$	204.357 g/mol		0.12
10.	Epiglobulol	$C_{15}H_{26}O$	222.372 g/mol		0.18
11.	Tau.-Muurolol	$C_{15}H_{26}O$	*mol/g 222.372*		0.93
12.	Cubenol	$C_{15}H_{26}O$	222.372 g/mol		0.90
13.	Isoaromadendrene epoxide	$C_{15}H_{24}O$	220.356 g/mol		1.41

14.	Globulol	$C_{15}H_{26}O$	222.372 g/mol		2.18
15.	Humulane-1,6-dien-3-ol	$C_{15}H_{26}O$	222.372 g/mol		0.81
16.	Caryophyllene	$C_{15}H_{24}$	204.357 g/mol		0.35
17.	Aristolene	$C_{15}H_{24}$	204.357 g/mol		3.20
18.	Alpha-Ylangene	$C_{15}H_{24}$	204.357 g/mol		0.60
19.	2(1H) Naphthalenone, 3,5,6,7,8,8a-hexahydro-4,8adimethyl- 6-(1-methylethenyl)-	$C_{15}H_{22}O$	218.334 g/mol		0.19
20.	beta-Vatirenene	$C_{15}H_{22}$	202.341 g/mol		8.61
21.	Alpha - Cedrene	$C_{15}H_{24}$	204.357 g/mol		0.56
22.	Selin-6-en-4α-ol	$C_{15}H_{26}O$	222.366g/mol		2.99
23.	Gamma-himachalene	$C_{15}H_{24}$	204.357 g/mol		1.14
24.	Valerenol	$\boldsymbol{C}_{15}H_{24}O$	220.356 g/mol		19.88
25.	Alpha -Guaiene	$C_{15}H_{24}$	204.357 g/mol		0.34
26.	Alpha – Gurjunene	$C_{15}H_{24}$	204.357 g/mol		0.57
27.	Longiverbenone	$C_{15}H_{22}O$	218.34 g/mol		3.46

28.	Alpha -Longipinene	$C_{15}H_{24}$	204.357 g/mol		0.84
29.	Alpha –Amorphene	$C_{15}H_{24}$	204.357 g/mol		0.565
30.	bete-Copaene	$C_{15}H_{24}$	204.357 g/mol		0.39
31.	Nootkatone	$C_{15}H_{22}O$	*mol/g 218.34*		0.57
32.	Isolongifolene, 4,5-dehydro	$\boldsymbol{C}_{15}H_{22}$	*mol/g 202.341*		0.17

Conclusion

Vetiver has been in use since ancient times for its aromatic roots and its essential oil. The complex composition of the essential oils and the variety of chemical structures of their constituents are responsible for a wide range of biological activities. The major components of vetiver oil were Valerenol, Beta-Vatirenene, Longiverbenone, Germacrene D, Aristolene and Selin-6-en-4-o.

Acknowledgements

The authors are highly grateful to the and Department of Medicinal and Aromatic Crops, Department of Spices and Plantation Crops, and Department of Biochemistry, Tamil Nadu Agricultural University, Coimbatore, Tamil Nadu, India for providing technical assistance during the research programme.

Reference

1. Bhuiyan NI, Chowdhury JU, Begum J. Essential oil in roots of *Vetiveria zizanioides* (L.) Nash ex small from Bangladesh. Bangladesh J Bot. 2008; 37(2):213-215.
2. Chahal KK, Bhardwaj U, Kaushal S, Sandhu AK. Chemical composition and biological properties of *Chrysopogon zizanioides* (L) Roberty syn. *Vetiveria zizanioides* (L) Nash-A Review, Indian Journal of Natural product and resources. 2015; 6(4):251-260.
3. Champagnat P, Figueredo G, Chalchat JC. A study on the composition of commercial V*etiveria zizanioides* oils from different geographical origins. J Essent. Oils Res. 2006; 18:416-422.
4. Chou ST, Lai CP, Lin CC, Shih Y. Study of the chemical composition, antioxidant activity and anti-inflammatory activity of essential oil from *Vetiveria zizanioides.* Food Chem. 2012; 134:262–268.
5. Chowdhury AR, Kumar D, Lohani H. GC-MS analysis of essential oils of *Vetiveria zizanioides* (Linn.) Nash roots. Fragrances and Flavours Association of India Journal. 2002; 4:33-35.
6. Dalton PA, Smith RJ, Truong PNV. Vetiver grass hedges for erosion control on a cropped flood plain: I Hedge hydraulics. Agr Water Manag. 1996; 31:91-104.
7. Kadarohman A, Ratnaningsih Eko S, Dwiyanti G, Lela Lailatul, K, Kadarusman E *et al*. Quality and chemical composition of organic and non-organic vetiver oil. Indo. J. Chem, 2014; 14(1):43-50.
8. Kim HJ, Chen F, Wang X, Chung HY, Jin Z. Evaluation of antioxidant activity of vetiver (*Vetiveria zizanioides* L.) oil and identification of its antioxidant constituents. J Agric. Food Chem. 2005; 53(20):7691-7695.
9. Lai RK, Sharma JR, Naqvi AA. Deve1opment of new varities- Dharni, Gulabi and Kesari of vetiver (*Vetiveria zizanioides*). J Med Aron, Plaizi Sd. 1998; 20:1067-1070.
10. Lavania UC. Other uses and utilization of vetiver: vetiver oil. The Third International Vetiver Conference, Guangzhou, China, 2003.
11. Mallavarapua GR, Kodakandla V, Syamasundarb S, Rameshc, Bhaskaruni R, Rajeswara R. Constituents of South Indian Vetiver Oils. Natural Product Communications. 2012; 7:223-225.
12. Marriott P, Shellie R, Fergeus J, Ong R, Morrison P. High resolution essential oil analysis by using comprehensive gas chromatographic methodology. Flav Fragr J. 2000; 15:225-239.
13. Pripdeevech P, Wongpornchai S, Promsiri A. Highly Volatile Constituents of *Vetiveria zizanioides* roots grown under different cultivation conditions. *Molecules.* 2006; 11:817-826.
14. Putrawan I, D GA, Eric F. Simple vacuum distillation of vetiver oil from smallholders for quality improvement, Global Journal of Research in Engineering. 2015; 15(3):1-7.
15. Yanto E, Agustian Egi, Sulaswatty A. Simple Purification of Vetiver Oil by Multiglass Plate System for Quality Improvement. J Kim Terap Indones. 2016; 18(2):124-131.