

<b>Analytical Report</b>	
Title	<b>Citronella Java</b> Essential Oil Profile by GC-MS
Report No.	SE-37270-7
Issue Date	August 31, 2015
Notebook reference	III-29-75
Contributors:	
Quote No.	
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**Primary Aim**

To identify GC amendable volatile organic compounds present in submitted **Cardamom** essential oil sample.

**Samples**

The sample arrived as clear liquid with characteristic odor labeled as "Citronella Java lot 11229-b17".

**Experimental:**

1. Oil was dissolved in methanol to concentration of ~0.1%, 1 ul injected into the GC injector port.
2. GC conditions:
 

Injector temperature:	250 C
Initial oven temperature:	80 C
Ramp	10 C/min
Final temperature	220 C
Final temperature hold	5 min

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### 3. MS parameters

Ionization and ion polarity	EI+
Scan rate	2 scans/sec
Mass range	35-350 Da
Ion source temperature	150C
Transfer line temperature	280C

4. GC-MS analysis. Waters/Micromass Quatro GC mass spectrometer interfaced to a ThermoElectron Trace gas chromatograph was utilized for the analysis. 30m 0.25 mm ID DB-5 column was used to separate components. Carrier gas was helium at 1.1 ml/min with split ratio of 50.

### 5. Data treatment.

For each sample, a set of target components was identified with the aid of the AMDIS software<sup>1</sup>. The components were identified using the NIST mass spectral library<sup>2</sup>.

## Deliverables

1. GC-MS chromatogram. GC-MS chromatogram is shown in Appendix I.
2. Appendix II lists library search results.
  - RT Retention Time, time in minutes at which the compound elutes out of column
  - CAS. CAS registry number or EPA number.
  - Name. IUPAC or common name of identified compound.
  - Area. Peak area of a component in %% to total ion count

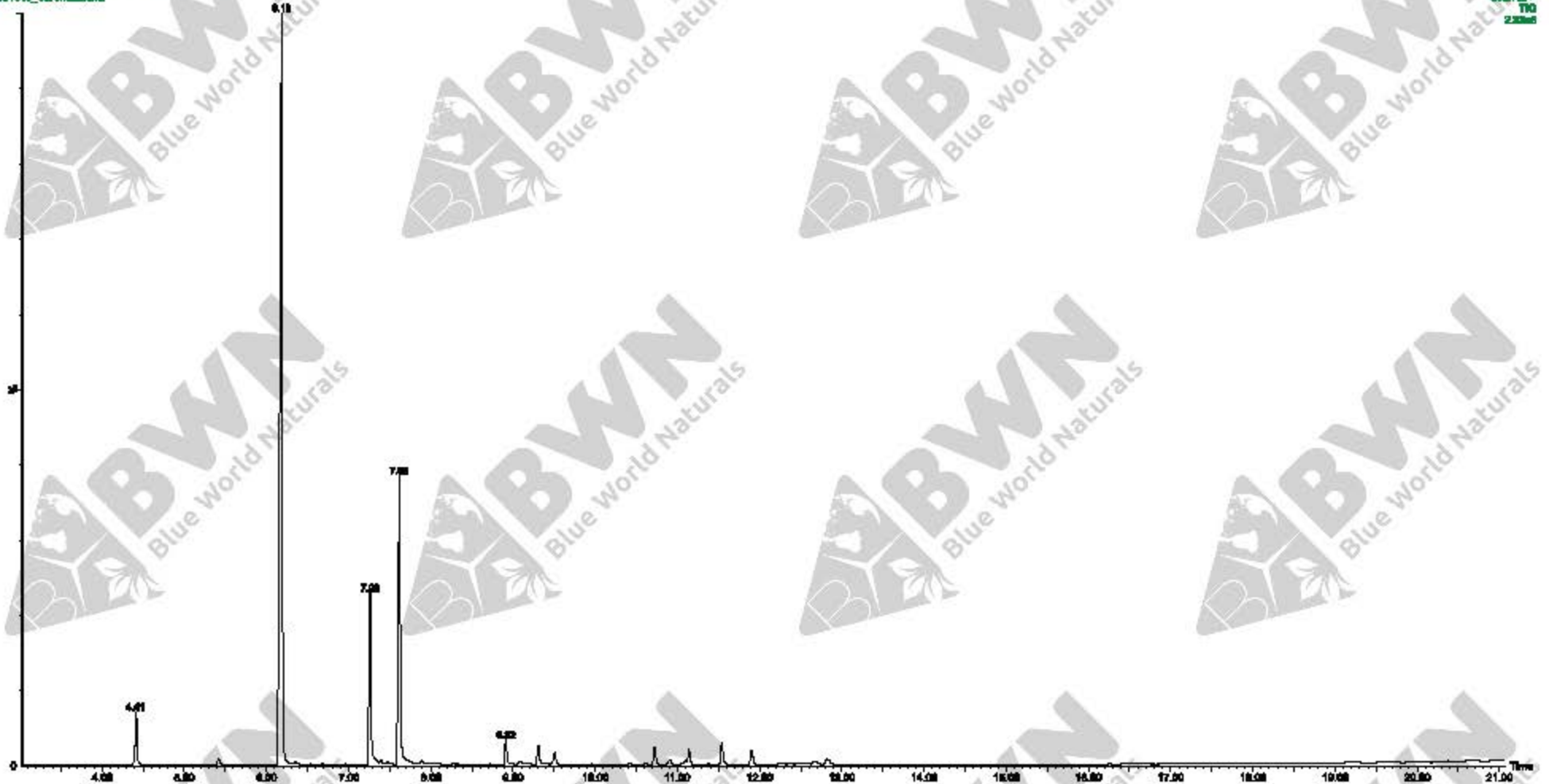
1 <http://chemdata.nist.gov/mass-spc/amdis/>

2 <http://www.nist.gov/srd/nist1a.cfm>

APPENDIX I  
Citronella Java  
GC-MS Chromatogram

# Sample "Citronella Java"

Citronella Java on DB-5 Int 11226-b17  
081016\_CitronellaJava



APPENDIX II  
Citronella Java  
Identified Compounds

## Citronella Java

CAS	Name	R.T.	Area
138863	Limonene	4.393	3.3
29765853	2-Cyclopenten-1-one, 2,3,5-trimethyl-4-methylene-	5.203	0.0
78706	1- $\beta$ -Octadien-3-ol, 3,7-dimethyl-	5.398	0.5
2385775	6-Octenal, 3,7-dimethyl-, (R)-	6.162	54.2
89792	Cyclohexanol, 5-methyl-2-(1-methylethenyl)-, [1R-(1 $\alpha$ ,2 $\beta$ ,5 $\alpha$ )]	6.332	0.3
106230	6-Octenal, 3,7-dimethyl-	6.652	0.0
106230	6-Octenal, 3,7-dimethyl-	6.659	0.0
112312	Decanal	6.952	0.0
1117619	6-Octen-1-ol, 3,7-dimethyl-, (R)-	7.238	11.4
106229	6-Octen-1-ol, 3,7-dimethyl-	7.375	0.2
106263	2- $\beta$ -Octadienal, 3,7-dimethyl-, (Z)-	7.459	0.1
106263	2- $\beta$ -Octadienal, 3,7-dimethyl-, (Z)-	7.505	0.0
106252	2- $\beta$ -Octadien-1-ol, 3,7-dimethyl-, (Z)-	7.596	18.2
141275	2- $\beta$ -Octadienal, 3,7-dimethyl-, (E)-	7.866	0.2
2497214	4-Hexen-3-one	8.696	0.0
2792394	2- $\beta$ -Octadiene, 2,6-dimethyl-	8.892	1.7
97530	Eugenol	9.06	0.3
105873	2- $\beta$ -Octadien-1-ol, 3,7-dimethyl-, acetate, (E)-	9.283	1.4
110823682	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-	9.489	0.8
59131134	1,5-Hexadiene, 2,5-dimethyl-3-methylene-	9.938	0.0
3338554	1,3-Octatriene, 3,7-dimethyl-, (Z)-	10.396	0.1
23986745	1- $\beta$ -Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyl)-, [s-(E,E)]-	10.598	0.1
23986745	1- $\beta$ -Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyl)-, [s-(E,E)]-	10.704	1.2
31983229	Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1 $\alpha$ ,4 $\alpha$ ,8 $\alpha$ )	10.89	0.4
110823682	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-	11.045	0.1
483750	Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-	11.084	0.2
483761	Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)-	11.124	1.1
31983229	Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1 $\alpha$ ,4 $\alpha$ ,8 $\alpha$ )	11.364	0.1
639996	Cyclohexanemethanol, 4-ethenyl- $\alpha$ , $\alpha$ ,4-trimethyl-3-(1-methylethenyl)-, [1R-(1 $\alpha$ ,3 $\alpha$ ,4 $\beta$ )]	11.523	1.6
72120504	1-Hydroxy-1,7-dimethyl-4-isopropyl-2,7-cyclodecadiene	11.885	1.0
74753007	1,4-Hexadiene, 3,3,5-trimethyl-	12.223	0.0
1209718	2-Naphthalenemethanol, 1,2,3,4,4a,5,6,7-octahydro- $\alpha$ , $\alpha$ ,4a- $\beta$ -tetramethyl-, (2R-cis)-	12.54	0.1
54324037	(+)-Epi-bicyclosesquiphellandrene	12.633	0.1
19912620	.tau.-Muurolool or isomer	12.663	0.2
513235	Bicyclo[3.1.0]hexan-3-ol, 4-methyl-1-(1-methylethyl)-	12.663	0.3
19912620	.tau.-Muurolool or isomer	12.799	0.5
63891612	2-Naphthalenemethanol, 2,3,4,4a,5,6,7,8-octahydro- $\alpha$ , $\alpha$ ,4a- $\beta$ -tetramethyl-, [2R-(2 $\alpha$ ,4 $\alpha$ ,8 $\beta$ ,8 $\beta$ )]	12.826	0.1

Citronella Java

473154 2-Naphthalenemethanol, decahydro- $\alpha,\alpha,4a$ -trimethyl-8-methylene-, [2R-(2 $\alpha$ ,4 $\alpha$ ,8 $\alpha$ (S))]-

12.826

0.2