Volatile Constituents of Faham (*Jumellea fragrans* (Thou.) Schltr.)

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The volatiles of faham leaves, a flavoring and medicinal plant of the Indian Ocean, have been analyzed by GC/MS. Besides the main compound, coumarin, 99 minor components were identified after enrichment with a preparative capillary chromatograph. The presence of diterpenes (kaurenes and phytadienes) was confirmed using GC/FTIR. This study represents the first description of the volatile fraction of faham. A sensory evaluation of the leaves of faham used in rums and infusions is also given.

INTRODUCTION

Jumellea fragrans (Thou.) Schltr., commonly called faham (Lavergne, 1989), is an endemic orchid of the Mascarene Islands in the Indian Ocean. The plant is 10–15 cm in length and grows on trees in tropical forests at altitudes between 400 and 1500 m.

It is often used as a medicinal plant against asthma, influenza, and infant gastroenteritis as well as for its digestive and anti-inflammatory properties (Vera et al., 1990). Faham, which has a flavor similar to that of tonka beans, is also often used as a flavoring in rums for local consumption.

The faham flavor develops within the leaves of the plant during the drying process. Originally, the green leaves are almost odorless and yield approximately 5 times fewer volatiles than the final product. However, as the leaves brown, chemical changes (probably enzymatic) occur, which result in the formation of the characteristic faham flavor. To date, only one reference on faham (Liefertova, 1985) has been published in the chemical literature. No information on the composition of volatiles has been given.

EXPERIMENTAL PROCEDURES

Sample Preparation. Green plants were bought at a local market and submitted to drying and browning at room temperature. The leaves were ground just prior to analysis. Eleven grams of ground leaves was put into a modified Likens–Nickerson steam distillation extractor (Godefroot et al., 1981), together with 600 mL of distilled, degassed water and 30 mL of redistilled CH_2Cl_2 (Merck 6054). The extraction was carried out for 5 h under nitrogen to prevent oxidation. The solvent was then dried over $MgSO_4$ and evaporated to about 100 μL under a N_2 stream before gas chromatography.

A blank Likens–Nickerson experiment using water and CH_2Cl_2 did not exhibit a significant peak after concentration in similar proportions.

Gas Chromatography. For all chromatography, a Hewlett-Packard 5890 gas chromatograph equipped with either an FID, MS, or FTIR detector was used. Except for preparative injections, separations were achieved on either a nonpolar or a polar column. The nonpolar column was a 50 m × 0.2 mm i.d. × 0.33 μm film thickness fused silica capillary column (50 m × 0.32 mm i.d. × 1.05 μm for GC/FTIR experiments) coated with cross-linked methylsilicone (HP1, Hewlett-Packard). The polar column was a 60 m × 0.25 mm i.d. × 0.25 μm film thickness fused silica column coated with cross-linked poly(ethylene glycol) (Supelcowax TM10, Supelco).

The oven temperature was held at 20 °C for 0.5 min, ballistically increased to 60 °C, and programmed at 4 °C/min to 220 °C for the polar phase column or 250 °C for the nonpolar phase column. The program was then held at isotherm until the end of the run.

The injector temperature was 250 °C, and 0.2 μL was injected in splitless mode. Detector temperatures were 275 °C for the FID, 220 °C for the MS, and 220 °C for the FTIR.

Helium was used as the carrier gas at the rates of 0.5 and 1.2 mL/min for nonpolar columns of 0.2 and 0.32 mm i.d., respectively, and 0.7 mL/min for polar columns.

Linear indices were calculated from the injection of an *n*-alkane reference series (C_5–C_{28}) (Van den Dool and Kratz, 1963) and compared to the indices reported in the literature or to those of our own libraries determined from authentic samples.

For the semiquantitation of volatiles, 0.105 g of 6-methylcoumarin was added to the sample flask as internal standard just before the Likens–Nickerson extraction. Apart from coumarin, other peaks were only estimated by assuming an arbitrary response factor of 1.

Mass Spectrometry. Electron impact mass spectrometry was performed on either a Hewlett-Packard 5995 or 5988 mass spectrometer with the capillary column directly interfaced into the ionization source operating at 70-eV ionization energy. The mass spectra of the compounds detected were compared with those in the Wiley library and in our user-generated libraries. The acquisitions in the negative chemical ionization mode were collected on the HP 5988 Model with a 1:1 mixture of CH_4/N_2O as reactant gas yielding hydroxyl ions, under a source pressure of 1 Torr.

Fourier Transformed Infrared Spectrometry. On-line GC/FTIR spectra were collected from a Hewlett-Packard Model 5965A using a gold-coated light pipe (1 mm × 110 mm) operating at 220 °C with an auxillary N_2 flow of 1.5 mL/min. The detector was an MCT type operating between 800 and 4000 cm^{-1} with a resolution of 8 cm^{-1}.

Preparative Chromatography. A Hewlett-Packard Model 5890 gas chromatograph, modified by the Gerstel Co. (Mühlheim a.d. Ruhr, Germany), was used for all preparative chromatography. The system is fully computer controlled and allows bidimensional separations as well as the collection of up to six fractions in traps cooled with liquid N_2 (Rijks, 1990; Werkoff et al., 1991).

The separation was achieved on two fused capillary columns connected in series. The first column was 5 m × 0.53 mm i.d. × 2.65 μm film thickness, and the second was 30 m × 0.53 mm i.d. × 0.88 μm film thickness. Both were coated with cross-linked methylsilicone (HP1, Hewlett-Packard). One hundredth of the flow was split to an FID detector after each column. The outlet of the second column was connected to a collector.

A total of 12 injections of 6 μL each was achieved with a

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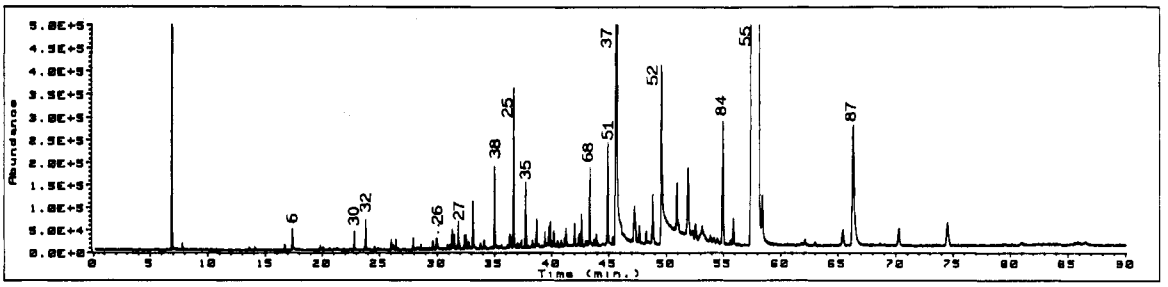


Figure 1. GC/MS chromatogram of the faham dry leaves extract before enrichment of the minor compounds (polar phase). Numbers refer to Table I.

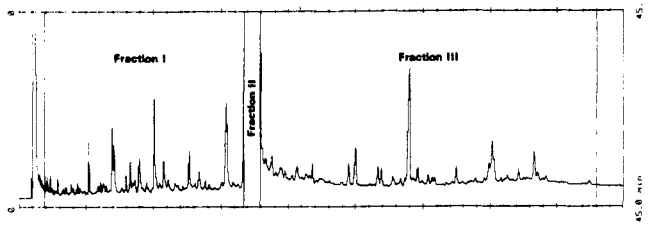


Figure 2. Preparative chromatogram of the faham dry leaves indicating the three fractions collected.

programmed injector temperature ranging from 150 to 250 °C at 12 °C/s. Helium was used as the carrier gas at a flow of 10 mL/min. A makeup of 1 mL/min between the injector and the first column and a second makeup of 1 mL/min between the two columns were also used. The oven temperature was increased from 60 to 250 °C at 5 °C/min. Fractions were collected at −35 °C.

Phytadienes Preparation. Phytadienes were obtained by dehydrating phytol with anhydrous oxalic acid in refluxing dioxane (Johnstone and Quan, 1963). Only three hydrocarbon peaks were obtained which were identified as phytadienes (m/z 278). Retention indices were, respectively, 1840, 1862, and 1881; IR maxima were found at 1631, 1596, 990, and 898 cm^{-1} (peak 1), 1643, 1597, 988, and 906 cm^{-1} (peak 2), and 1641, 1609, 987, and 897 cm^{-1} (peak 3). All of these values were in agreement with published data for phytadienes I–III (Blumer and Thomas, 1965; Marion, 1970; Hites, 1974).

RESULTS AND DISCUSSION

The volatile compounds of the dry, ground leaves were isolated in a Likens–Nickerson extractor (Experimental Procedures), and the organic extract was concentrated. From the chromatogram presented in Figure 1, only 15 peaks were concentrated enough for mass spectral identification. Since the coumarin represented 85% of the volatile fraction, an enrichment of all other minor components was necessary to obtain recognizable mass spectra.

The Max Planck Institute has recently developed a fully automated chromatograph for preparative isolation using capillary columns. This device, commercialized by the Gerstel Co., proved its efficiency for the enrichment of the faham extract. The chromatogram was cut into three fractions (Figure 2). The collected fractions 1 and 3 were reinjected in the GC/MS or the GC/FTIR. Fraction 2, which only contained coumarin, was reinjected only in the GC to verify the purity.

The enrichment of the 12 injections of 6 μL each is illustrated in Figures 3 and 4. Peaks from fraction 3 were observed to tail when reinjected on a polar column.

Overall, 99 components (Table I) were identified from the faham leaves, and their presence was confirmed in the raw extract even though their low abundances did not originally allow spectral recognition.

All compounds were quantified on the basis of the chromatogram obtained before enrichment so as to exclude the possible disparities of the recovery yields. Thus, minor peaks representing less than 0.03% of the total area were not estimated.

Phytadienes. Attention was given to the phytadienes (Figure 5) because the mass spectra of their isomeric forms were quite similar and their retention indices were not well differentiated.

Infrared and retention data of four isomers found in zooplankton have been published (Blumer and Thomas, 1965). A GC/FTIR experiment was performed on fraction 3, using the selected wavelengths 3095 cm^{-1}, which is common to phytadienes I–III (vinyl groups), 1598 cm^{-1}, related to conjugated dienes (Johnstone and Quan, 1963), and 900 cm^{-1}, for the CH bending of monosubstituted vinyl groups (Morin et al., 1989).

In the index region of the phytadienes on the apolar phase, three absorption maxima were detected for the three wavelengths at indices 1844, 1868, and 1893 (Figure 6).

Negative CI-MS exhibited quasi molecular ions at 277 Da, confirming the occurrence of diterpenes. The IR spectra corresponding to these indices (Figure 7) indicated the presence of a vinyl group (988 and 900 cm^{-1}) and a conjugated system (1642 and 1600 cm^{-1}) (Morin et al., 1989). This only leads to three phytadiene isomers (Figure 5). Blumer differentiated isomer III from the others since it absorbed at 1600 (our experiment 1609 cm^{-1}) instead of 1590 cm^{-1} (our experiment 1596–1597 cm^{-1}). Similarly, isomers I and III absorbed at 893–896 cm^{-1} (our experiment 898–897 cm^{-1}), whereas isomer II was shifted to 904 cm^{-1} (our experiment 906 cm^{-1}). At last, isomer I presented a higher abundance at mass 68 (78%) indicating that the MacLafferty rearrangement was not hindered by the diene substituents as with isomers II and III.

All of these observations were confirmed by comparing the indices and the IR and MS spectra with those of authentic phytadienes prepared by dehydrating phytol.

The assignment of phytadienes II and III to cis and trans structures was based on Blumer's observation and could not be confirmed by the spectral data.

The dehydration of phytol into neophytadiene (phytadiene I) (Johnstone and Quan, 1963) did not seem to occur using our isolation or chromatographic conditions, because phytol was detected in the absence of phytadienes when faham stems were used. According to Johnstone, the migration of the diene system toward the center of the chain does not occur to a significant extent, and it should lead to the formation of various cyclohexenes.

Kaurenes and Other Diterpenes. Although their MS spectra are better differentiated than those of phytadienes, the identification of kaurenes and other diterpenes required further IR confirmation because of the low resolution of GC peaks in this region on nonpolar columns and tailing on the polar phases. Hibaene, kaur-15-ene, kaur-16-ene, and atisirene tallied well with the literature values for retention indices (Table I) as well as for MS and IR spectra (Table II).

Table I. Volatile Compounds Identified in Leaves of Faham

peak	compound	retention index polar[a]	retention index nonpolar[b]	concn,[c] ppm	peak	compound	retention index polar[a]	retention index nonpolar[b]	concn,[c] ppm
1	2,3-butanedione	976	*d*	–	50	4-hydroxynonanoic acid, lactone	2051	1334	–
2	pyridine	1183	*d*	–	51	eugenol	2180	1344	40
3	heptanal	1188	*d*	–	52	dihydrocoumarin	2314	1350	31
4	isopentanol	1199	*d*	–	53	β-damascenone	*d*	1368	–
5	pentanol	1241	*d*	–	54	methyl eugenol	2018	1377	–
6	3-hydroxy-2-butanone	1292	*d*	–	55	coumarin	2358	1414	10500
7	hexanol	1345	*d*	–	56	β-ionone	1958	1480	8
8	tetradecane	1396	*d*	–	57	5-hydroxy-2-decenoic acid, lactone	2246	1499	22
9	heptanol	1449	*d*	–	58	pentadecane	1496	1517	9
10	nonanol	1654	*d*	–	59	dihydroactinidiolide	2372	1532	20
11	2-tridecanone	1797	*d*	–	60	dodecanoic acid	*d*	1556	–
12	4-hydroxyoctanoic acid, lactone	1939	*d*	–	61	hexadecane	1596	1617	5
13	2-ethylhexanoic acid	1965	*d*	–	62	heptadecene	*d*	1680	3
14	5-hydroxyoctanoic acid, lactone	1993	*d*	–	63	2-pentadecanone	1997	1684	–
15	3(2*H*)-benzofuranone (tentative)	2008	*d*	–	64	heptadecane	*d*	1702	4
16	tridecanol	2076	*d*	–	65	benzyl benzoate	2505	1743	–
17	nonanoic acid	2113	*d*	–	66	tetradecanoic acid	*d*	1762	6
18	decanoic acid	2220	*d*	–	67	octadecane	1800	1802	–
19	isopentanol	*d*	642	–	68	6,10,24-trimethyl-2-pentadecanone	2096	1848	32
20	butoxyethanol	1402	887	–	69	phytadiene I	1954	1852	33
21	benzaldehyde	1540	938	11	70	benzyl salicylatel	*d*	1857	–
22	*p*-cymene	*d*	974	–	71	pentadecanoic acid	*d*	1860	–
23	2-pentylfuran	*d*	984	–	72	phytadiene II	1984	1871	13
24	benzofuran	1521	986	9	73	phytadiene III	1996	1883	37
25	benzyl alcohol	1883	1017	63	74	methyl hexadecanoate	2220	1914	–
26	phenylacetaldehyde	1659	1019	7	75	hibaene	*d*	1951	18
27	salicylaldehyde	1701	1024	33	76	isophytol	2282	1956	–
28	2,5-epoxymegastigma-4,9-diene (tentative)	*d*	1042	4	77	sandaracopimaradiene	*d*	1965	7
					78	hexadecanoic acid	*d*	1966	96
29	octanol	1552	1059	3	79	ethyl hexadecanoate	*d*	1985	9
30	*cis*-linalool oxide (furanoid)	1446	1068	4	80	icosane	2000	2006	–
31	2-methoxyphenol	1873	1071	4	81	kaur-15-ene	*d*	2018	440
32	*trans*-linalool oxide (furanoid)	1475	1082	–	82	heptadecanoic acid	*d*	2038	–
33	nonanal	1398	1089	–	83	atisirene	*d*	2054	–
34	linalool	*d*	1091	–	84	kaur-16-ene	*d*	2061	250
35	phenylethanol	1921	1099	11	85	methyl linolenate	*d*	2084	–
36	3,5,5-trimethyl-2-cyclohexene-1,4-dione	1708	1117	6					
					86	heneicosane	2100	2104	–
37	2-vinylphenol	2203	1141	200	87	*trans*-phytol	2611	2125	27
38	4-hydroxyacetophenone	1790	1146	61	88	octadecanoic acid	*d*	2137	–
39	heptanoic acid	*d*	1160	–	89	ethyl linolenate	*d*	2153	–
40	*cis*-linalool oxide (pyranoid)	1743	1164	–	90	docosene (isomer?)	*d*	2198	–
41	*trans*-linalool oxide (pyranoid)	1763	1167	–	91	docosane	*d*	2205	–
42	α-terpineol	*d*	1187	–	92	kauren-19-ol (tentative)	*d*	2290	81
43	β-cyclocitral	*d*	1202	–	93	tricosane	2298	2306	20
44	4-phenylbutanone	1876	1228	–	94	tetracosene (isomer?)	*d*	2396	–
45	decanol	1720	1244	–	95	tetracosane	2398	2402	–
46	octanoic acid	*d*	1256	–	96	pentacosane	2498	2503	32
47	vitispirane	*d*	1276	–	97	hexacosene (isomer?)	*d*	2594	–
48	geranial	*d*	1287	–	50	hexacosane	*d*	2601	170
49	4-hydroxy-(*Z*)-non-6-enoic acid, lactone	2102	1323	–	99	heptacosane	*d*	2701	

[a] Linear retention index calculated on Supelcowax TM 10 phase. [b] Linear retention index calculated on HP1 phase. [c] Estimated quantity. A dash indicates a concentration too low for quantitation in the raw extract. [d] Not observed on this column, or tailing peak without possibility of index calculation.

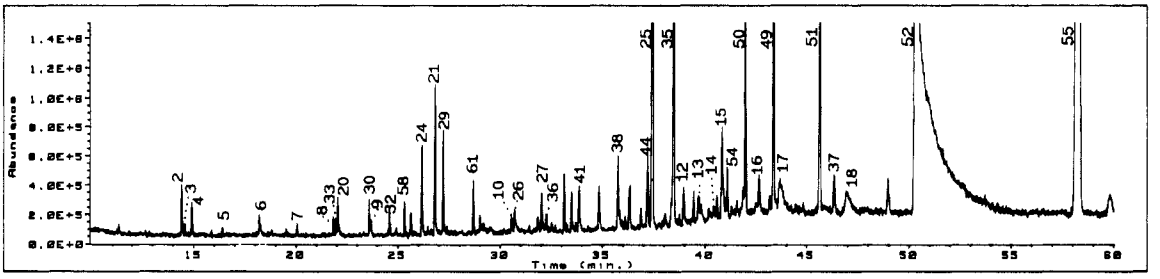
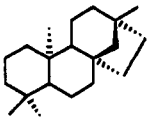
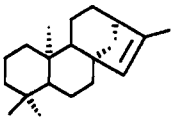
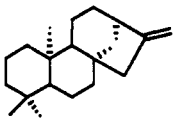
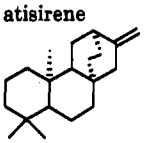
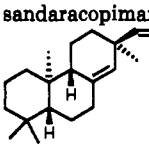


Figure 3. Fraction I of enrichment of the minor compounds by preparative capillary GC (polar phase). Numbers refer to Table I.

Although sandaracopimaradiene eluted with hexadecanoic acid, the characteristic absorption bands of the *gem*-dimethyl and of the vinyl groups supported this identification as well as the retention index (Lorimer and Weavers, 1987). However, further to the lack of reference of IR spectrum in the literature, this identification could not be confirmed with certainty.

Sensory Evaluation. A comparative taste test was performed by an expert panel between a raw rum and a rum held for 5 months with a macerated branch of faham.

Table II. IR Data for Kaurenes and Related Compounds

compound	IR abs found, cm^{-1}	IR abs lit., cm^{-1}	EI-MS fragments
hibaene 	1391 1373 746	1388[a] 1365[a] 750[a]	41 (100), 55 (58), 91 (59), 93 (58), 105 (65), 106 (51), 119 (40), 122 (38), 134 (68), 135 (61), 148 (28), 150 (26), 272 (34)
kaur-15-ene 	3031 1647 817	3045[b] 1650[b] 810[b]	41 (71), 55 (41), 94 (100), 106 (49), 119 (23), 147 (13), 163 (14), 187 (9), 229 (6), 272 (15)
kaur-16-ene 	3074 1659 1386 1366 879	3070[c] 1655[c] 1385[c] 1365[c] 872[c]	41 (100), 55 (38), 79 (40), 91 (62), 105 (42), 125 (26), 147 (23), 213 (14), 229 (18), 257 (27), 272 (19)
atisirene 	3073 1651 1392 1372 880	3081[c] 1650[c] 1386[c] 1368[c] 875[c]	41 (57), 55 (100), 83 (73), 91 (39), 98 (99), 257 (73), 272 (6)
sandaracopimaradiene 	3074, 3025 1660 1465 1378 1388, 1362	str CH of monosubst vinyl str C=C vinyl bend CH_2 and CH_3 bend CH_3 bend CH of *gem*-dimethyl	81 (46), 95 (41), 105 (33), 136 (52), 137 (100), 257 (38), 272 (22)

[a] As liquid film (Briggs and White, 1975). [b] MacMillan and Walker (1972). [c] In CCl_4 (Briggs and White, 1975).

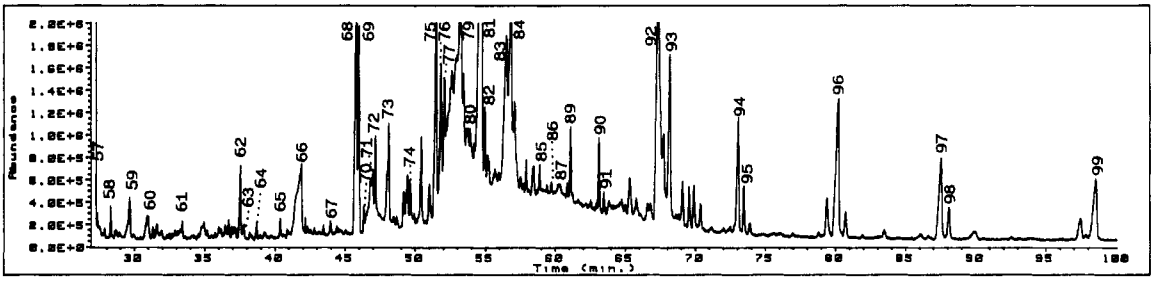


Figure 4. Fraction III of the enrichment of the minor compounds by preparative GC (nonpolar phase). Numbers refer to Table I.

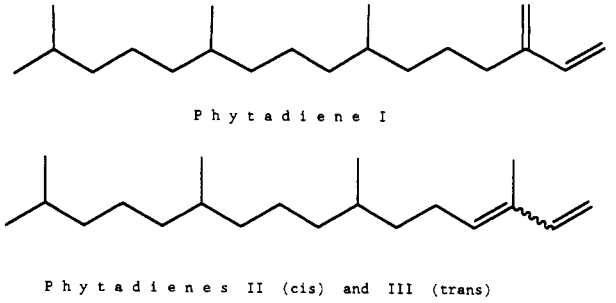


Figure 5. Assigned structures of phytadienes I–III.

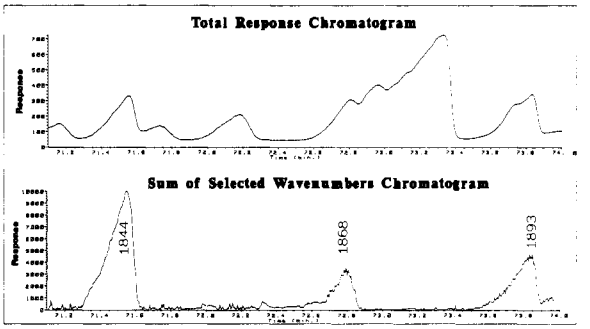


Figure 6. FTIR and selected wavenumber chromatogram of the phytadiene absorptions giving the corresponding retention indices.

Compared to the original rum sample, the modified rum was described as "old rum" and warm, with an undernote of green olive.

Since faham is also used for traditional medicinal purposes as an aqueous infusion, leaves were also tasted in this form. Aside from its typical coumarin character, the faham flavor was bitter with honey and artichoke notes. The aroma of the infusion was reminiscent of tea.

CONCLUSIONS

Because FTIR detectors are less sensitive than MS detectors, their use is limited for the evaluation of minor peaks. The use of the preparative capillary GC was observed to dramatically enhance the capabilities of IR and MS detectors, particularly when the trapping and the

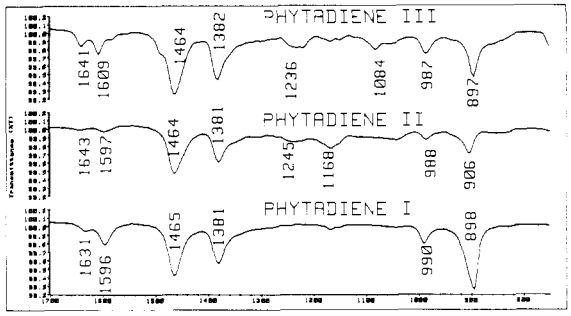


Figure 7. GC/FTIR spectra in the 800–1700-cm^{-1} region of phytadienes.

control of the instrument were fully automated for routine applications. The identification of almost 100 components was attributed to the use of this preparative tool.

These results also indicate that in addition to its medicinal value and potential as an alternative flavoring to tonka beans, faham also has a potential in perfumery due to the high level of coumarin detected in the extracts of the dried leaves. However, addition of faham in food should take into account its coumarin content, which is regulated in many countries (IOFI, 1990). Although the use of faham is currently limited due to a reduction in growing area, the aromatic and medicinal properties of the plant make faham a viable consideration for future cultivation.

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Registry No. 2,3-Butanedione, 431-03-8; pyridine, 110-86-1; heptanal, 111-71-7; isopentanol, 123-51-3; pentanol, 71-41-0; 3-hydroxy-2-butanone, 513-86-0; hexanol, 111-27-3; tetradecane, 629-59-4; heptanol, 111-70-6; nonanol, 143-08-8; 2-tridecanone, 593-08-8; 4-hydroxyoctanoic acid lactone, 104-50-7; 2-ethylhexanoic acid, 149-57-5; 5-hydroxyoctanoic acid lactone, 698-76-0; 3(2*H*)-benzofuranone, 7169-34-8; tridecanol, 112-70-9; nonanoic acid, 112-05-0; decanoic acid, 334-48-5; isopentanal, 590-86-3; butoxyethanol, 111-76-2; benzaldehyde, 100-52-7; *p*-cymene, 99-87-6; 2-pentylfuran, 3777-69-3; benzofuran, 271-89-6; benzyl alcohol, 100-51-6; phenylacetaldehyde, 122-78-1; salicylaldehyde, 90-02-8; octanol, 111-87-5; *cis*-linalool oxide (furanoid), 5989-33-3; 2-methoxyphenol, 90-05-1; *trans*-linalool oxide (furanoid), 34995-77-2; nonanal, 124-19-6; linalool, 78-70-6; phenylethanol, 60-12-8; 3,5,5-trimethyl-2-cyclohexene-1,4-dione, 1125-21-9; 2-vinylphenol, 695-84-1; 4-hydroxyacetophenone, 99-93-4; heptanoic acid, 111-14-8; *cis*-linalool oxide (pyranoid), 14009-71-3; *trans*-linalool oxide (pyranoid), 39028-58-5; α-terpineol, 98-55-5; β-cyclocitral, 432-25-7; 4-phenylbutanone, 2550-26-7; decanol, 112-30-1; octanoic acid, 124-07-2; vitispirane, 65416-59-3; geranial, 141-27-5; 4-hydroxy-(*Z*)-non-6-enoic acid lactone, 76710-90-2; 4-hydroxy-nonanoic acid lactone, 104-61-0; eugenol, 97-53-0; dihydrocoumarin, 119-84-6; β-damascenone, 23726-93-4; methyleugenol, 93-15-2; coumarin, 91-64-5; β-ionone, 79-77-6; 5-hydroxy-2-decenoic acid lactone, 54814-64-1; pentadecane, 629-62-9; dihydroactinidiolide, 17092-92-1; dodecanoic acid, 143-07-7; hexadecane, 544-76-3; heptadecene, 26266-05-7; 2-pentadecanone, 2345-28-0; heptadecane, 629-78-7; benzyl benzoate, 120-51-4; tetradecanoic acid, 544-63-8; octadecane, 593-45-3; 6,10,14-trimethyl-2-pentadecanone, 502-69-2; phytadiene isomer 1, 504-96-1; benzyl salicylate, 118-58-1; pentadecanoic acid, 1002-84-2; phytadiene isomer 2, 100210-90-0; methyl hexadecanoate, 112-39-0; hibaene, 2359-73-1; isophytol, 505-32-8; sandaracopimaradiene, 1686-56-2; hexadecanoic acid, 57-10-3; ethyl hexadecanoate, 628-97-7; icosane, 112-95-8; kaur-15-ene, 5947-50-2; heptadecanoic acid, 506-12-7; atisirene, 20230-48-2; kaur-16-ene, 562-28-7; methyl linolenate, 112-63-0; heneicosane, 629-94-7; *trans*-phytol, 150-86-7; octadecanoic acid, 57-11-4; ethyl linolenate, 1191-41-9; docosene, 29730-67-4; docosane, 629-97-0; kauren-19-ol, 2300-11-0; tricosane, 638-67-5; tetracosene, 36731-16-5; tetracosane, 646-31-1; pentacosane, 629-99-2; hexacosene, 64808-91-9; hexacosane, 630-01-3; heptacosane, 593-49-7.