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Volatile Components from Mango (*Mangifera indica* L.) Cultivars

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The volatile components of 20 mango cultivars were investigated by means of simultaneous distillation−extraction, GC, and GC-MS. Three hundred and seventy-two compounds were identified, of which 180 were found for the first time in mango fruit. The total concentration of volatiles was ∼18−123 mg/kg of fresh fruit. Terpene hydrocarbons were the major volatiles of all cultivars, the dominant terpenes being δ-3-carene (cvs. Haden, Manga amarilla, Macho, Manga blanca, San Diego, Manzano, Smith, Florida, Keitt, and Kent), limonene (cvs. Delicioso, Super Haden, Ordoñez, Filipino, and La Paz), both terpenes (cv. Delicia), terpinolene (cvs. Obispo, Corazón, and Huevo de toro), and α-phellandrene (cv. Minin). Other qualitative and quantitative differences among the cultivars could be demonstrated.

KEYWORDS: Mango cultivars; *Mangifera indica* L.; volatile compounds; GC-MS

INTRODUCTION

Mango (*Mangifera indica* L.) is one of the most important and popular of tropical fruits, mainly due to its attractive flavor. Several hundreds of cultivars are grown in various parts of the world and are known to vary markedly in their flavor characteristics (*1*).

The volatile constituents of mango have been extensively investigated. More than 300 compounds have been identified as free forms (*2*−*4*) and ∼70 compounds as glycosidically bound compounds (*5*−*7*). The variability in volatile compounds of mango has been reported to depend on the cultivar (*8*−*16*), maturity stage of the fruit (*11*, *17*−*19*), part of the fruit (*20*), and processing (*21*−*24*).

Sample preparation has also been reported to cause a variation in volatile compounds of the fruit (*25*). The methods used to isolate volatile compounds in mango included solvent extraction (*6*, *24*), vacuum steam distillation followed by solvent extraction (*23*, *26*, *27*), simultaneous distillation−extraction (*8*, *10*, *11*, *13*, *16*, *17*, *28*), static headspace (*14*, *29*), dynamic headspace concentration (*9*, *12*), solid-phase extraction (*30*), and headspace solid-phase microextraction (*19*, *20*).

The present work was aimed at investigating the volatile compounds of some Cuban mango cultivars and then comparing results with those already documented for other cultivars.

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MATERIALS AND METHODS

Materials. Batches of fresh ripe mangos from at least two trees were collected over a 1-month period during the peak of the normal harvest (May−June) in the National Botanic Garden in Havana, Cuba. Twenty cultivars were selected: Delicioso, Haden, Super-Haden, Manga amarilla, Macho, Manga blanca, Ordoñez, Obispo, Corazón, Delicia, Filipino, Huevo de toro, San Diego, Manzano, Smith, Florida, Minin, La Paz, Keitt, and Kent. The stage of maturity was measured by external color and firmness. The mangos were analyzed when fully ripe (normally yellow-red colors and soft to the touch) in the following manner: Six fruits free from any skin damage were selected from each batch. The peeled fruits were then sliced and pureed immediately in a commercial blender. Pure reference standards of acetaldehyde, ethanol, 1-propanol, ethyl acetate, isobutanol, 1-butanol, 1-penten-3-ol, 1-penten-3-one, 2,3-pentanedione, pentanal, 3-pentanone, 2-ethylfuran, 3-pentanol, propyl acetate, ethyl propanoate, acetoin, methyl butanoate, methyl methacrylate, 3-methyl-1-butanol, (*E*)-3-penten-2-one, 2-methyl-1-butanol, pyridine, (*E*)-2-pentenal, ethyl 2-methylpropanoate, methyl (*E*)-crotonate, 1-pentanol, (*Z*)-2-penten-1-ol, toluene, 3-methyl-2-buten-1-ol, methyl 2-methylbutanoate, 2,4-pentanedione, 2-methylpropanoic acid, butyl formate, butanoic acid, hexanal, ethyl butanoate, 2-methyltetrahydrofuran-3-one, butyl acetate, ethyl methacrylate, 2-furfural, isovaleric acid, ethyl (*E*)-2-crotonate, ethyl 2-methylbutanoate, ethyl 3-methylbutanoate, (*Z*)-3-hexenol, methyl 3-hydroxybutanoate, 1-hexanol, ethylbenzene, 4-heptanone, 3-methylbutyl acetate, cyclohexanol, 2-heptanone, *o*-xylene, cyclohexanone, propyl butanoate, heptanal, butyl propanoate, 2,5-dimethylpyrazine, γ-butyrolactone, methyl hexanoate, 2,5-hexanedione, ethyl 3-hydroxybutanoate, ethyl tiglate, (*E*)-2-heptenal, 5-methyl-2-furfural, 1-heptanol, 1-octen-3-ol, β-pinene, hexanoic acid, methyl furoate, 2-octanone, butyl butanoate, 2-carene, ethyl hexanoate, octanal, δ-3-carene, *p*-cymene, 1,8-cineole, benzyl alcohol, salicylal-

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dehyde, cyclohexyl acetate, phenylacetaldehyde, butyl isopentanoate, γ-hexalactone, (*E*)-2-octenal, 2,5-dimethyl-4-methoxy-3(2*H*)-furanone, acetophenone, 1-octanol, ethyl maltol, diallyl disulfide, allyl hexanoate, terpinolene, *p*-cymenene, methyl benzoate, ethyl sorbate, ethyl heptanoate, tetrahydrolinalool, linalool, nonanal, α-fenchol, 2-phenylethanol, isophorone, methyl octanoate, ethyl 3-hydroxyhexanoate, isobutyl tiglate, phenylacetonitrile, camphor, isopulegol, menthone, (*E*)-2-nonenal, borneol, benzyl acetate, *p*-tolyl acetate, ethyl benzoate, menthol, methyl phenylacetate, octanoic acid, 4-methylacetophenone, (*Z*)-3-hexenyl butanoate, butyl hexanoate, α-terpineol, methyl salicylate, hexyl butanoate, methylchavicol, ethyl octanoate, *trans*-dihydrocarvone, verbenone, decanal, α-methylcinnamaldehyde, octyl acetate, β-cyclocitral, 1,2-benzothiazole, *cis*-carveol, pulegone, cuminaldehyde, carvone, ethyl phenylacetate, isopentyl hexanoate, *p*-anisaldehyde, geraniol, 2-phenylethyl acetate, benzyl propanoate, γ-octalactone, (*E*)-2-decenal, ethyl salicylate, citronellyl formate, nonanoic acid, (*E*)-anethole, bornyl acetate, safrole, thymol, ethyl nonanoate, carvacrol, undecanal, 4-vinylguaiacol, 4-propylanisole, methyl decanoate, allyl phenylacetate, piperonal, methyl anthranilate, 4-acetylanisole, benzyl butanoate, α-terpinyl acetate, citronellyl acetate, eugenol, benzyl isothiocyanate, γ-nonanalactone, neryl acetate, butyl benzoate, methyl (*E*)-cinnamate, decanoic acid, geranyl acetate, hexyl hexanoate, isobutyl phenylacetate, octyl isobutanoate, benzyl isopentanoate, diphenyl ether, ethyl decanoate, methyl eugenol, allyl cyclohexylpropanoate, α-(*E*)-ionone, methyl undecanoate, 2-phenylethyl butanoate, geranylacetone, ethyl (*E*)-cinnamate, γ-decalactone, geranyl propanoate, (*E*)-β-ionone, valencene, δ-decalactone, ethyl undecanoate, (*E*)-methyl isoeugenol, tridecanal, methyl dodecanoate, (*E*)-nerolidol, γ-undecalactone, dodecanoic acid, caryophyllene oxide, 2-phenylethyl tiglate, ethyl dodecanoate, tetradecanal, benzophenone, methyl tridecanoate, (*Z*)-jasminaldehyde, (*Z*)-3-hexenyl salicylate, γ-dodecalactone, tridecanoic acid, ethyl tridecanoate, 2-pentadecanone, methyl tetradecanoate, benzyl benzoate, (*Z*)-9-tetradecenoic acid, (*Z*)-9-tetradecenoic acid, ethyl tetradecanoate, benzyl salicylate, methyl hexadecanoate, methyl palmitoleate, hexadecanoic acid, ethyl hexadecanoate, methyl linoleate, methyl oleate, methyl octadecanoate, oleic acid, ethyl linoleate, ethyl linolenate, octadecanoic acid, ethyl oleate, and ethyl octadecanoate were purchased from Aldrich (Steinheim, Germany). (*E*)-2-Hexenal, α-pinene, camphene, 6-methyl-5-hepten-2-one, α-terpinene, limonene, *o*-tolualdehyde, *cis*-linalool oxide, *p*-tolualdehyde, terpinen-4-ol, β-caryophyllene, α-humulene, tetradecanoic acid, pentadecanoic acid, hexadecanol, methyl linolenate, and ethyl pentadecanoate were purchased from Fluka (Buchs, Switzerland). Diethyl ether was purchased from Merck (Darmstadt, Germany).

Sample Preparation. Two hundred grams of fruit pulp was homogenized with 600 mL of distilled water; 0.2 mg of methyl nonanoate was added as standard, and the volatile compounds were isolated by means of simultaneous distillation−extraction using 25 mL of diethyl ether (previously redistilled and checked as to purity) for 1 h. The aroma extract was dried over Na_2SO_4 and concentrated to 0.6 mL in a Kuderna-Danish evaporator with a Vigreux column and then to 0.2 mL with a gentle nitrogen stream.

Gas Chromatography and Gas Chromatography−Mass Spectrometry Analysis. A Konik 2000 GC, equipped with a 30 m × 0.25 mm × 0.25 μm film thickness DB-5 (J&W Scientific, Folsom, CA) or a 30 m × 0.25 mm × 0.25 μm film thickness DB-Wax (J&W Scientific) fused-silica capillary column with a flame ionization detector was used. Injector and detector temperatures were both 250 °C. Oven temperature was held at 60 °C for 10 min and then raised to 280 °C at 4 °C/min and held for 40 min. Carrier gas (hydrogen) flow rate was 1 mL/min. The retention times of a series of straight-chain alkanes (C_6−C_{24}) were used to calculate the retention indices for all identified compounds and for reference standards. Quantitative determinations were carried out according to the internal standard method without consideration of isolation yields and calibration factors for all compounds. Recovery with the method was determined by the standard addition technique applied to a sample. The analytes [α-pinene, limonene, ethyl hexanoate, 1-hexanol, (*Z*)-3-hexenol, ethyl octanoate, β-caryophyllene, and α-terpineol] were added at two different concentrations. The average recoveries were ∼89−102%, and their relative standard deviations were <10%.

GC-MS analyses were performed on a Hewlett-Packard series 6890 gas chromatograph linked to an HP-5973 mass-selective detector, with the following conditions: a 30 m × 0.25 mm i.d., 0.25 μm film thickness HP-5MS (Agilent, Palo Alto, CA) fused silica capillary column; temperature program, 60 °C (2 min), raised at 4 °C/min to 250 °C (20 min); injector temperature, 250 °C; carrier gas, He adjusted to a flow rate of 1 mL/min; split mode, 1:10; EIMS, electron energy, 70 eV; ion source and connecting parts temperature, 230 °C. Compounds were preliminarily identified by use of NIST, Wiley, NBS, and our own mass spectra libraries, as well as MS data from the literature (*31*, *32*), and then the identities of most were confirmed by comparison of their linear retention indices with those of reference standards or with published data (*32*).

Sensory Analysis. A sensory panel, with six assessors selected on the basis of their performance, was organized. The ranking difference method (*33*) was used to compare the aroma intensity from whole fresh fruit of each variety with that of cv. Corazón, which is considered to be one of the Cuban mango cultivars having the most intense flavor.

RESULTS AND DISCUSSION

Taking into account that sample preparation causes a variation in volatile compounds and that we were interested in comparing our results with earlier studies, most using simultaneous distillation−extraction, we decided to use this isolation method. In addition, this method is often the best way to get the highest recoveries from a wide range of compounds (*34*).

Volatile constituents of 20 mango cultivars were isolated using a well-established method, basically identical to those previously used in this laboratory for other fruits (*35*−*37*). The concentrated extracts were found, on appropriate redilution, to possess the characteristic mango aroma of each cultivar. **Table 1** lists the volatile compounds identified by comparison of their mass spectra and retention indices with those of authentic samples and with published data. In total, 372 volatile compounds were identified, of which 180 were newly identified as mango fruit constituents.

The quantitative data in **Table 1** show that in total ∼18−123 mg of volatile compounds was obtained per kilogram of fresh fruit (excluding skin and stone) for the 20 cultivars.

Members of the sensory panel easily distinguished between the cv. Corazón and the other cultivars (significant at 0.05% level). Because Corazón has the higher amount of volatiles, with 122.46 mg/kg, these results confirm the findings of the sensory panel of this cultivar having the most intense flavor. Nevertheless, these data alone do not necessarily mean that cv. Corazón has a stronger aroma or flavor, because relative odor intensities of different compounds will affect the total perceived intensity.

Previous analyses of fresh mango pulp using similar techniques yielded the following range of concentrations: 60 μg/kg for Venezuelan fruit (*28*); 41.2 and 88.8 mg/kg for Alphonso and Baladi cultivars, respectively (*8*); 57 mg/kg for Alphonso cultivar (*27*); 251, 422, and 628 μg/kg for Sri Lankan cultivars (Jaffna, Willard, and Parrot, respectively) (*10*); 72 and 54 mg/kg for Tommy Atkins and Keitt cultivars from Florida (*11*); and 39, 58, and 70 mg/kg for Bizcochuelo, Super Haden, and Corazón cultivars, respectively (*13*).

Terpene hydrocarbons, as in most previously studied mango cultivars (*6*, *8*, *10*−*17*, *19*, *27*, *28*), were by far the dominant volatiles in the studied cultivars. Fifty terpenes were identified, comprising 19 monoterpenes and 32 sesquiterpenes, all of which have been previously reported in this fruit (*3*, *4*) except for 13 of them [*p*-1,3,8-menthatriene, α-cedrene, 9-*epi*-(*E*)-caryophyllene, selina-4,11-diene, *ar*-curcumene, α-zingiberene, viridiflorene, β-bisabolene, *cis*-calamenene, β-sesquiphellandrene, α-cadinene, α-calacorene, and germacrene B].

Table 1. Volatile Compounds Identified in 20 Cultivars[a] of Mango Fruits (Milligrams per Kilogram

compound	ID[b]	RI[c]	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
acetaldehyde	A	528	t[d]	t	t	t	t	t	t	t	t	t	t	t	t	t	t	t	t	t	t	t
ethanol	A	537	t	1.23	t	t	t	t	t	t	–	t	t	t	t	t	t	t	t	t	–	–
1-propanol[e]	A	568	–[f]	–	–	0.64	–	–	–	–	t	–	–	–	–	–	–	–	–	–	–	–
ethyl acetate	A	605	t	t	–	0.55	t	0.51	t	4.90	t	–	t	t	t	t	t	–	t	t	–	–
isobutanol	A	622	t	t	t	0.55	t	t	t	–	t	–	–	–	–	–	–	–	–	–	t	–
1-butanol	A	668	0.70	0.44	t	4.26	t	1.65	0.28	0.55	1.79	t	0.44	0.28	0.10	0.71	0.23	0.28	t	t	0.46	0.56
1-penten-3-ol[e]	A	673	0.20	0.11	0.06	t	0.11	t	–	0.25	–	t	t	t	0.03	0.27	0.09	0.11	0.04	0.12	t	0.38
1-penten-3-one[e]	A	678	t	0.11	0.06	t	0.11	t	–	0.25	–	0.25	–	–	0.03	–	–	–	0.04	0.12	–	–
2,3-pentanedione[e]	A	696	–	t	t	t	–	t	–	t	–	–	–	t	0.03	–	t	t	t	t	t	t
pentanal	A	698	–	t	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
3-pentanone	A	700	t	–	t	t	t	–	–	–	–	t	–	–	–	t	–	–	–	–	t	–
2-ethylfuran[e]	A	702	–	–	t	t	t	t	0.02	t	–	t	t	t	t	–	–	–	t	t	t	t
3-pentanol	A	710	t	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
propyl acetate[e]	A	712	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	t	–	–	–
ethyl propanoate	A	714	–	t	t	t	t	–	–	–	–	–	–	–	–	t	–	–	t	–	0.08	0.13
acetoin	A	720	0.13	0.14	0.03	0.37	–	0.16	0.07	0.27	1.32	0.16	0.10	0.09	0.12	0.17	0.55	0.11	0.02	0.37	–	–
methyl butanoate	A	724	t	0.04	t	–	–	0	0.11	t	t	–	–	0.09	0.01	t	0.11	t	t	t	t	–
methyl methacrylate[e]	A	732	–	–	t	–	–	–	–	–	–	–	–	–	–	–	0.32	–	t	–	–	–
3-methyl-1-butanol	A	734	0.54	0.16	0.09	0.77	0.09	0.19	0.48	0.48	0.47	0.15	0.19	0.40	0.09	0.10	–	0.10	0.01	0.23	0.21	0.15
(*E*)-3-penten-2-one	A	735	–	t	t	t	t	–	–	0.18	–	–	–	–	–	–	t	–	–	t	–	–
2-methyl-1-butanol[e]	A	736	t	t	t	0.55	0	–	t	–	–	–	0.19	0.40	0.02	0.10	–	0.10	t	t	–	0.13
pyridine	A	753	t	t	t	0.08	t	0.02	–	0.03	0.08	0.05	0.04	t	t	t	t	t	t	0.07	t	t
(*E*)-2-pentenal	A	754	0.02	–	0.03	0.09	0.03	–	–	–	t	t	–	–	–	t	–	0.02	0.01	t	t	0.06
ethyl 2-methylpropanoate	A	755	0.02	0.06	t	–	t	–	0.02	t	0.08	–	t	t	0.02	0.02	0.03	–	0.01	t	0.03	–
methyl (*E*)-crotonate[e]	A	756	–	t	0	–	t	–	0.03	t	0.14	–	–	–	t	t	0.06	t	t	t	t	t
1-pentanol	A	768	t	t	0.14	0.13	–	–	–	t	–	–	t	–	–	0.08	–	–	t	0.08	t	–
(*Z*)-2-penten-1-ol	A	769	0.12	0.15	t	t	–	–	–	–	–	–	–	–	0.09	0.10	–	t	t	t	t	t
toluene	A	773	–	t	t	t	t	–	0.02	t	t	t	0.05	t	t	–	0.05	t	0.04	t	0.08	0.10
3-methyl-2-buten-1-ol	A	778	t	t	t	–	–	–	t	t	–	–	–	–	–	–	–	t	–	t	–	–
methyl 2-methylbutanoate[e]	A	780	t	t	t	–	t	–	t	–	t	–	–	t	–	–	–	–	t	–	t	–
(*E*,*E*)-1,3,5- heptatriene[e]	C	781	–	–	–	–	–	–	–	–	–	t	t	–	t	–	t	t	t	–	0.02	0.08
2,4-pentanedione	A	783	–	–	t	–	–	–	–	0.09	–	–	–	–	–	–	–	0.04	0	–	–	–
2-methylpropanoic acid[e]	A	785	–	t	t	–	–	–	0.06	–	–	–	–	–	t	–	–	–	0.02	–	–	–
butyl formate[e]	A	787	–	–	t	–	–	–	–	t	–	t	–	–	–	–	t	–	–	–	t	–
butanoic acid	A	790	t	t	0.02	t	0.07	–	t	t	0.35	–	–	0.07	0.04	–	–	t	t	0.10	–	–
2-propylfuran[e]	C	792	t	t	t	–	t	–	–	t	–	t	–	–	–	0.01	–	t	–	t	t	t
hexanal	A	800	–	t	0.02	–	0.14	–	–	0.22	–	–	–	–	–	–	–	–	–	–	–	0.07
ethyl butanoate	A	802	0.44	1.25	0.02	0.52	t	0.06	2.96	–	4.89	0.08	0.10	4.19	0.26	0.22	2.08	0.34	0.02	0.13	0.06	–
2-methyltetrahydrofuran-3-one[e]	A	804	–	–	–	–	t	–	–	–	–	–	–	–	–	–	–	–	–	–	t	–
2-ethoxypropane[e]	A	806	–	–	–	t	–	–	–	t	–	–	–	–	–	–	–	–	–	t	t	–
butyl acetate	A	812	0.05	–	t	0.03	–	t	0.51	–	–	0.14	–	–	–	t	–	–	–	–	t	–
ethyl methacrylate	A	814	t	0.09	0.06	0.03	0.04	0.04	t	0.52	1.22	0.14	0.02	0.49	0.12	0.27	2.49	0.15	0.01	0.39	0.10	0.37
2-furfural	A	830	0.03	0.04	0.04	0.04	0.02	–	0.01	0.04	0.06	0.02	0.02	0.02	0.05	t	0.02	0.02	0.02	0.01	0.01	0.03
isovaleric acid	A	834	t	t	–	t	t	t	–	t	–	–	–	–	t	–	–	t	t	t	–	–
ethyl (*E*)-crotonate	A	835	0.03	0.13	0.01	0.03	0.15	0.03	0.93	0.11	1.55	0.03	0.02	0.56	0.06	0.29	1.49	0.08	0.01	0.19	0.02	0.02
(*Z*)-2-hexenal[e]	A	841	0.03	t	–	–	t	–	–	–	–	–	–	–	–	–	–	–	–	–	–	t
ethyl 2-methylbutanoate	A	842	t	t	–	t	t	–	0.03	–	t	t	t	t	t	t	t	–	–	–	–	–
2-methylbutanoic acid	C	846	–	t	–	–	–	–	–	–	–	–	–	–	–	–	–	t	–	t	–	–
ethyl 3-methylbutanoate	A	847	–	t	–	–	–	–	0.03	–	–	–	–	–	–	–	0.04	t	–	–	t	–
(*E*)-2-hexenal	A	854	0.53	0.10	0.05	0.04	0.37	–	–	0.25	0.29	0.09	0.34	0.03	0.05	0.08	t	0.06	0.01	0.09	t	0.07
(*Z*)-3-hexenol	A	857	0.62	0.09	0.02	0.24	0.08	–	0.06	1.02	0.09	t	0.89	0.03	0.04	0.10	0.19	0.20	0.13	0.20	0.05	0.30
methyl 3-hydroxybutanoate[e]	A	858	–	–	–	–	–	–	–	–	0.09	–	–	–	–	–	t	–	–	–	–	–
1-hexanol	A	867	0.12	0.04	0.02	0.23	t	–	0.04	0.25	0.17	0.08	0.09	–	0.02	0.16	0.02	0.04	0.01	0.05	0.02	0.04
ethylbenzene	A	868	t	t	0.02	–	t	–	t	t	–	t	0.05	0.03	t	–	0.02	t	t	t	t	–
4-heptanone[e]	A	869	–	t	–	–	0.01	–	–	t	t	–	–	–	t	–	t	t	–	–	–	–
3-methylbutyl acetate	A	876	t	t	t	t	t	–	t	t	–	t	t	0.02	t	–	t	t	t	t	0.01	–
2-methylbutyl acetate	B	880	t	t	t	–	–	–	t	–	–	–	–	–	t	–	t	–	–	–	–	–
cyclohexanol[e]	A	886	0.03	–	0.04	–	t	–	t	–	–	0.04	0.03	0.01	0.02	0.02	t	0.01	t	0.01	0.01	–
2-heptanone	A	889	0.02	0.01	0.02	t	t	–	0.01	0.03	–	0.02	0.01	t	0.02	0.02	0.03	0.01	0.01	0.02	0.01	0.01
styrene[e]	C	890	t	t	t	t	t	t	t	t	t	–	–	–	t	–	–	0.01	t	t	0.01	–
o-xylene	A	894	t	0.02	0.04	t	t	–	t	–	–	t	0.04	–	–	–	t	t	–	t	t	–
cyclohexanone	A	895	t	t	t	–	–	–	t	t	–	0.05	t	–	0.01	t	t	0.01	t	–	–	–
propyl butanoate	A	896	0.02	0.01	–	–	–	–	0.03	t	t	t	–	0.01	0.01	t	0.03	–	–	0.03	t	–
heptanal	A	899	0.01	t	t	0.02	0.01	–	t	0.03	–	t	–	–	t	t	0.01	t	0.01	t	0.01	0.02
methyl 2-hydroxybutanoate[e]	C	907	–	t	t	t	t	–	–	–	t	–	–	–	–	–	t	t	–	–	–	–
santolina triene[e]	B	908	–	–	–	–	–	–	–	t	–	–	–	–	–	–	–	t	–	–	t	–
butyl propanoate[e]	A	910	t	t	0.01	t	t	–	t	t	–	t	t	t	t	t	0.02	t	–	t	t	–
2,5-dimethylpyrazine[e]	A	911	t	t	t	t	t	–	–	–	–	t	t	t	0.01	t	t	t	–	0.01	t	–

Table 1. (Continued)

compound	ID[b]	RI[c]	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
γ-butyrolactone	A	915	t	–	–	t	–	–	–	–	t	–	–	–	–	–	–	–	–	–	–	–
tricyclene	B	923	–	–	–	t	–	–	–	–	t	–	–	–	–	–	–	–	–	–	t	–
methyl hexanoate	A	924	0.01	0.01	0.01	–	0.04	–	0.02	0.15	–	0.02	t	0.04	0.02	0.02	0.08	0.06	t	0.09	0.01	–
α-thujene	B	931	t	t	t	0.04	t	–	t	t	t	t	–	–	–	t	t	t	t	t	t	–
2,5-hexanedione[e]	A	933	–	–	t	–	t	–	–	–	–	–	–	–	t	t	t	–	–	–	–	–
α-pinene	A	939	0.11	0.15	0.06	1.40	0.62	0.16	0.58	4.15	4.73	0.18	0.02	1.17	0.11	0.40	0.59	0.20	0.03	0.23	0.25	0.08
ethyl 3-hydroxy-butanoate	A	945	t	t	t	0.01	t	–	t	–	2.67	t	t	t	t	t	0.97	t	t	t	–	t
ethyl tiglate	A	949	t	0.01	t	–	–	–	0.08	–	0.47	–	t	t	t	–	0.06	t	–	t	–	–
2,3-dihydro-3-(1-methylpro-pyl)furan[e]	C	950	–	0.02	t	–	–	–	0.02	–	–	–	–	–	–	–	0.02	t	–	t	–	t
α-fenchene	B	951	–	–	0.01	0.03	0.07	–	–	–	–	0.03	–	–	–	0.05	t	0.03	0.03	–	0.03	0.03
camphene	A	953	0.03	–	0.01	0.03	–	t	0.03	0.18	0.20	–	t	0.04	0.01	t	0.08	t	t	0.07	–	–
ethyl 3-oxobutanoate[e]	C	954	t	t	–	–	t	–	t	–	–	–	–	0	t	–	t	–	–	–	–	t
butyl isobutanoate[e]	A	955	t	t	t	t	–	–	0.02	–	–	–	–	0.01	t	t	t	–	–	t	0.02	t
(*E*)-2-heptenal	A	956	0.03	0.01	t	t	0.08	–	–	0.08	–	0.03	–	–	t	0.04	0.02	0.02	t	0.05	t	0.04
benzaldehyde	A	961	0.06	0.16	0.05	t	0.01	–	t	t	t	0.01	t	t	0.04	t	t	t	0.04	0.01	0.02	t
ethyl 2,3-epoxy-utanoate[e]	C	962	t	t	t	–	–	–	0.04	0.03	0.14	0.19	–	0.01	0.02	0.05	0.24	0.03	t	0.02	t	0.02
5-methyl-2-furfural	A	964	t	t	t	–	–	–	–	–	–	–	–	–	t	–	–	–	t	–	–	–
1-heptanol	A	969	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	0.01	–
sabinene	B	976	0.01	t	t	t	0.01	–	0.01	–	t	0.01	t	t	0.01	0.01	0.02	0.01	0.01	0.01	0.01	–
1-octen-3-ol[e]	A	978	t	t	0.01	t	t	–	0.01	0.04	–	0.01	t	t	0.01	t	0.02	t	t	0.01	t	–
β-pinene	A	980	0.02	0.01	0.01	0.24	0.04	0.02	0.45	0.55	0.40	0.02	0.01	0.12	0.01	0.02	0.04	0.02	0.01	0.02	0.02	t
hexanoic acid	A	981	t	–	0.01	t	t	–	t	t	–	–	–	t	t	–	–	0.02	t	t	–	–
methyl furoate[e]	A	983	–	t	t	–	–	–	–	–	–	–	–	–	t	–	–	–	–	–	–	–
6-methyl-5-hepten-2-one	A	985	t	0.01	t	t	t	–	t	t	–	t	t	t	0.01	t	t	t	0.01	–	–	–
dehydro-1,8-cineole[e]	C	990	–	–	–	–	–	–	–	t	t	–	–	–	–	–	–	–	t	t	t	t
myrcene	A	991	0.40	0.33	0.34	0.54	1.29	0.66	0.26	0.74	1.17	0.46	0.13	0.46	0.37	0.98	1.14	0.48	0.09	0.44	0.67	0.40
2-pentylfuran[e]	A	992	t	t	t	t	–	t	–	t	–	–	–	–	–	t	t	t	t	–	t	t
2-octanone[e]	A	992	t	t	–	t	–	t	t	–	–	–	t	–	t	–	–	–	–	t	t	–
ethyl (*Z*)-3-hexenoate[e]	B	993	–	–	–	–	–	–	–	–	t	–	–	–	–	–	t	–	–	t	–	–
butyl butanoate	A	994	0.09	0.03	–	0.11	–	0.12	0.04	t	0.19	0.05	0.01	0.05	–	0.03	t	0.01	–	0.02	t	0.03
2-carene	A	995	–	t	t	t	t	–	0.06	0.23	0.41	–	t	t	–	–	t	t	–	–	–	–
ethyl hexanoate	A	996	0.10	0.06	t	t	t	–	t	t	t	t	0.02	0.17	t	t	t	t	–	0.24	t	–
octanal	A	1001	–	–	–	t	–	–	–	–	–	–	–	–	–	–	t	–	–	–	–	–
α-phellandrene	A	1005	0.13	0.11	0.27	0.21	0.34	t	0.07	0.22	0.76	t	0.03	0.19	0.27	0.42	t	0.24	3.52	t	0.28	1.69
δ-3-carene	A	1011	4.13	6.90	3.39	10.68	18.75	14.92	0.40	3.82	4.14	6.58	0.11	1.17	3.49	17.29	16.85	9.04	2.23	4.80	9.72	4.07
1,4-cineole[e]	A	1016	t	0.11	0.09	0.17	t	–	t	–	–	0.10	0.07	t	t	0.26	t	0.13	t	t	t	–
α-terpinene	A	1018	0.21	t	t	t	0.24	t	0.23	0.53	1.95	t	t	0.61	0.09	t	0.28	t	0.02	0.10	0.16	0.03
p-cymene	A	1026	0.15	0.20	0.09	0.22	0.25	0.24	0.18	0.34	0.53	0.23	0.16	0.21	0.09	0.28	0.23	0.18	0.03	0.22	0.16	0.06
limonene	A	1031	8.41	4.23	4.59	6.26	7.94	10.20	7.78	8.69	10.49	6.22	4.73	9.01	7.49	9.38	14.53	6.88	1.01	8.17	7.82	1.34
1,8-cineole	A	1032	t	t	t	t	–	–	t	t	–	t	t	t	t	t	t	t	t	t	t	t
benzyl alcohol	A	1033	–	–	t	–	–	–	–	–	–	–	–	–	0.01	–	0.02	0.01	t	t	0.02	–
(*Z*)-β-ocimene	B	1040	0.02	0.01	0.01	t	0.02	–	0.01	0.03	0.10	0.01	0.01	0.03	0.01	0.02	0.03	0.01	t	0.02	0.02	t
salicylaldehyde[e]	A	1041	0.09	t	0.06	t	t	–	t	–	–	0.02	t	t	t	t	t	t	t	t	0	0.02
cyclohexyl acetate[e]	A	1043	0.03	0.02	0.06	0.03	0.02	t	0.02	0.02	t	0.03	0.04	0.02	0.05	0.03	0.05	0.02	0.01	0.03	0.03	t
phenylacetaldehyde	A	1044	t	0.06	t	t	0.05	–	–	0.03	0.07	t	t	t	0.04	0.05	0.04	0.04	0.01	0.07	0.02	t
butyl (*E*)-2-butenoate	C	1046	–	–	–	–	–	–	t	–	–	–	–	–	–	–	t	t	–	–	–	t
butyl isopentanoate[e]	A	1048	–	–	–	–	–	–	–	t	t	–	–	–	–	–	–	–	–	–	–	–
(*E*)-β-ocimene	B	1050	0.06	0.04	0.04	0.05	0.08	0.06	t	0.06	0.13	0.04	0.03	0.05	0.04	0.09	0.09	0.05	t	0.05	0.05	0.01
γ-hexalactone	A	1056	t	–	t	–	–	–	–	t	–	–	–	t	t	–	–	t	t	t	–	–
pentyl isobutanoate[e]	B	1057	t	t	t	–	t	0.49	t	t	t	–	t	t	t	–	t	–	–	t	t	t
γ-terpinene	A	1062	0.64	0.33	0.37	0.42	0.48	t	0.51	0.51	0.66	0.41	0.34	0.68	0.48	0.58	0.93	0.41	0.05	0.47	0.47	0.08
(*E*)-2-octenal[e]	A	1063	–	t	–	–	t	–	–	–	–	–	–	–	–	t	–	–	–	–	–	t
isopentyl butanoate	B	1064	t	t	t	t	t	t	t	t	t	–	t	t	t	t	–	t	t	t	t	–
2,5-dimethyl-4-meth-oxy-3(2*H*)-furanone	A	1065	t	t	0.01	0.09	0.04	–	t	1.88	0.59	t	t	t	0.01	t	0.01	t	–	0.02	–	–
acetophenone	A	1066	t	t	0.01	t	t	–	–	–	–	t	t	t	t	t	–	t	0.02	t	t	–
o-tolualdehyde[e]	A	1067	–	–	t	t	t	t	–	–	–	–	–	–	t	–	–	–	t	–	–	–
1-octanol	A	1070	–	–	t	t	–	–	–	–	–	t	–	–	t	–	–	0.01	–	–	t	–
cis-linalool oxide (furanoid)	A	1074	0.02	0.04	0.03	t	t	–	0.01	–	–	t	0.02	t	0.04	t	0.02	t	0.01	t	0.01	–
ethyl maltol[e]	A	1076	–	–	–	–	0.02	–	–	0.62	0.13	–	–	–	t	t	–	t	–	t	–	–
diallyl disulfide[e]	A	1077	t	t	t	t	t	–	0.01	–	–	t	t	t	t	t	t	0.01	–	t	0.01	–
p-tolualdehyde	A	1079	0.01	0.04	0.09	t	0.01	–	t	–	t	0.04	0.02	t	0.06	0.01	0.02	0.01	0.01	0.01	0.01	–
allyl hexanoate[e]	A	1080	t	t	t	t	t	–	t	–	–	t	–	t	t	t	t	t	t	t	0.05	0.02
terpinolene	A	1087	3.18	0.58	0.44	1.09	1.92	1.07	4.57	12.22	46.60	0.54	0.73	13.57	0.47	2.17	1.88	0.86	0.17	0.49	0.98	0.22
p-cymenene	A	1089	t	t	t	t	t	t	t	t	t	t	t	t	t	t	t	t	t	–	t	t
methyl benzoate	A	1091	0.15	0.21	0.27	0.15	0.14	t	0.13	0.21	0.36	0.09	0.05	0.15	0.30	0.16	0.31	0.12	0.01	0.14	0.14	0.01

Table 1. (Continued)

compound	ID[b]	RI[c]	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
ethyl sorbate[e]	A	1093	–	t	–	–	0.04	–	t	–	t	–	–	t	–	–	t	–	t	–	–	–
ethyl heptanoate[e]	A	1095	t	t	t	t	t	–	t	–	–	t	–	t	t	t	t	t	–	–	t	–
tetrahydrolinalool[e]	A	1097	–	t	t	–	–	–	–	–	–	t	t	–	–	–	–	–	–	–	–	–
linalool	A	1098	0.06	0.04	0.04	0.04	0.03	–	0.04	0.04	0.09	0.05	0.07	0.04	0.06	0.06	0.08	0.03	0.01	0.04	0.03	t
cis-thujone[e]	A	1102	t	t	0.04	t	0.04	–	–	t	–	–	–	–	–	–	–	–	t	–	t	t
nonanal	A	1103	0.03	0.02	0.01	0.03	t	–	0.02	t	–	0.04	t	t	0.03	0.02	0.04	0.03	0.01	0.03	0.02	0.02
p-1,3,8-menthatriene[e]	B	1110	0.01	t	–	t	0.01	–	0.01	0.08	0.38	0.01	t	0.03	0.01	0.01	0.02	0.01	0.01	–	0.01	–
α-fenchol[e]	A	1112	–	–	–	t	t	–	t	–	–	–	t	–	t	t	–	–	t	t	t	–
(*E*,*E*)-2,4-octadienal[e]	C	1113	t	t	t	t	t	–	t	–	–	–	–	–	–	–	t	t	t	t	t	t
2-phenylethanol	A	1114	0.02	t	0.06	t	0.02	–	–	t	–	t	–	–	0.04	–	0.01	0.01	t	0.03	0.02	t
isophorone[e]	A	1118	0.03	0.02	0.02	t	t	–	0.01	0.02	–	0.02	t	t	0.02	0.01	0.02	t	–	0.01	0.01	–
cis-*p*-2-menthen-1-ol[e]	C	1121	t	t	t	0.03	0.02	–	–	t	0.08	–	–	t	t	t	t	0.02	–	–	0.01	–
methyl octanoate	A	1126	0.02	0.01	0.02	0.02	0.02	–	0.01	0.03	0.03	0.02	t	0.01	0.02	0.02	0.04	0.02	0.01	0.02	0.02	–
ethyl 3-hydroxy-hexanoate	A	1133	t	0.01	–	t	–	–	t	–	0.04	–	–	–	0.01	t	0.06	–	–	t	t	–
isobutyl tiglate[e]	A	1136	t	t	–	–	–	–	0.01	–	–	–	–	–	–	–	0.02	t	–	–	–	t
phenylacetonitrile	A	1140	t	t	0.06	t	t	–	0.01	–	–	–	–	–	t	–	–	–	–	–	t	–
camphor[e]	A	1143	t	t	t	t	t	–	t	–	–	0.01	0.01	t	0.02	t	0.01	t	t	t	t	–
4-ketoisophorone	B	1142	t	–	t	t	t	–	–	–	–	t	–	–	t	t	t	0.01	–	t	–	t
trans-verbenol	B	1144	–	0.01	t	t	0.04	–	0.01	0.12	–	–	t	–	–	–	0.01	–	–	t	t	0.02
isopulegol[e]	A	1146	0.03	–	0.04	0.03	–	–	–	–	–	0.02	–	–	0.02	–	0.01	0.01	–	t	0.01	–
menthone[e]	A	1154	t	t	t	t	t	–	t	–	–	–	t	–	t	t	t	t	t	–	–	–
(*E*,*Z*)-2,6-nonadienal	C	1155	0.26	0.06	0.35	0.30	0.68	–	0.02	0.38	t	0.24	0.03	t	0.11	0.14	0.22	0.24	0.07	0.58	0.17	0.67
(*E*)-2-nonenal	A	1162	0.06	0.09	0.19	0.26	0.69	–	–	0.28	0.06	0.19	–	–	–	0.21	0.12	0.10	0.22	0.12	0.09	0.10
borneol[e]	A	1164	–	–	t	t	t	–	t	–	–	–	t	–	t	–	t	t	–	t	t	–
benzyl acetate	A	1165	–	t	t	t	–	–	–	–	–	–	t	–	0.03	–	t	–	–	0.02	0.01	–
p-tolyl acetate[e]	A	1166	t	t	t	–	–	–	–	–	–	–	–	–	–	–	t	–	–	t	t	–
p-mentha-1,5-dien-8-ol[e]	C	1167	t	0.02	t	0.08	0.08	–	t	0.04	0.11	0.02	–	–	–	0.08	0.11	0.03	0.02	t	t	t
ethyl benzoate[e]	A	1170	t	0.02	0.06	t	t	–	0.01	t	t	0.03	t	t	0.02	t	0.01	0.02	–	t	0.01	–
menthol	A	1173	–	–	–	–	t	–	–	–	–	–	t	–	–	–	0.01	–	–	–	–	–
terpinen-4-ol	A	1177	t	0.03	0.05	0.06	0.04	–	0.01	–	t	0.07	0.03	–	0.03	0.06	0.05	0.01	0.03	0.02	0.02	–
limonene-4-ol[e]	B	1178	0.06	t	t	t	t	–	0.02	–	0.36	–	–	0.08	–	–	–	–	–	t	t	–
methyl phenylacetate[e]	A	1179	t	t	t	–	–	–	t	–	–	–	–	–	t	–	–	–	–	–	–	–
m-cymen-8-ol	B	1180	t	0.01	t	–	0.02	–	–	–	–	0.02	t	–	–	0.02	0.06	0.02	–	0.01	–	–
octanoic acid	A	1180	t	–	t	–	t	–	–	–	–	0.07	–	–	–	–	t	–	t	–	–	–
4-methylacetophenone	A	1181	0.02	0.01	0.02	–	0.02	–	t	0.14	t	–	–	t	–	–	–	t	t	t	t	–
p-cymen-8-ol	B	1183	0.04	0.03	t	t	0.04	–	0.03	0.26	1.79	–	0.05	0.04	0.03	–	0.09	0.04	0.04	0.02	0.03	–
(*Z*)-3-hexenyl butanoate	A	1186	–	–	–	–	–	t	–	–	–	–	–	–	t	–	0.12	–	–	t	–	–
butyl hexanoate	A	1188	t	t	t	–	–	t	t	–	t	–	–	t	–	–	t	t	–	–	t	t
α-terpineol	A	1189	0.08	0.09	0.14	0.42	0.08	–	t	0.11	0.41	0.07	0.06	0.07	0.10	0.07	t	0.04	0.02	0.03	0.05	t
methyl salicylate[e]	A	1190	t	t	t	–	t	–	–	–	–	–	t	–	t	–	t	t	–	–	t	–
hexyl butanoate	A	1191	0.02	t	t	0.04	0.02	t	0.02	0.02	0.09	t	t	0.04	0.02	0.02	0.03	0.01	–	0.02	0.01	–
methylchavicol[e]	A	1195	0.03	0.06	0.15	0.04	0.02	–	0.03	0.04	0.07	0.05	0.06	0.04	0.09	0.06	0.08	0.03	0.03	0.05	0.03	0.01
ethyl octanoate	A	1196	0.06	0.04	t	0.07	0.05	t	0.06	0.11	0.72	0.05	0.02	0.19	0.06	0.10	0.24	0.06	t	0.06	0.05	t
trans-dihydrocarvone[e]	A	1200	–	–	t	–	–	–	–	–	–	–	–	–	–	–	–	–	t	–	–	–
verbenone	A	1204	–	0.02	–	t	t	–	–	–	0.06	–	–	–	–	–	–	–	–	–	–	–
decanal	A	1205	0.03	t	0.04	t	0.04	–	0.03	–	–	0.04	0.01	0.4	0.03	0.05	0.07	0.03	0.01	0.04	0.03	t
α-methylcinnamaldehyde[e]	A	1207	t	–	–	t	–	–	–	0.01	t	–	–	–	–	–	t	t	–	t	–	–
octyl acetate[e]	A	1211	0.01	0.01	t	0.01	0.02	–	0.01	0.01	t	0.01	t	t	0.01	0.02	0.03	0.01	–	0.01	0.01	–
β-cyclocitral[e]	A	1220	0.01	0.01	0.04	t	t	–	0.01	0.07	0.03	0.02	t	–	0.02	0.04	–	t	t	t	t	0.01
1,2-benzothiazole	A	1221	t	t	t	t	t	–	t	–	–	t	0.01	–	t	–	–	0.02	0.01	0.02	0.01	–
cis-carveol	A	1229	–	–	–	–	–	–	–	–	–	0.05	–	–	–	–	t	–	–	–	–	–
(*Z*)-3-hexenyl 2-methyl-butanoate[e]	C	1231	–	–	–	–	–	–	–	–	–	–	–	–	–	–	0.01	–	–	t	–	0.03
pulegone[e]	A	1237	t	–	t	–	–	–	–	–	–	–	–	–	0.02	–	–	–	–	–	t	–
cuminaldehyde	A	1239	0.01	0.03	0.07	t	0.01	–	0.02	–	–	0.03	0.02	0.03	0.02	0.03	0.21	0.01	t	0.03	0.01	–
neral	B	1240	t	t	t	t	0.01	–	–	t	–	t	t	–	t	0.02	t	t	t	–	t	–
carvone	A	1242	0.03	0.01	0.03	0.02	0.01	–	0.02	0.06	–	0.05	0.02	0.02	0.03	0.02	0.04	0.02	0.01	0.02	0.02	–
ethyl phenylacetate	A	1244	t	t	t	t	0.01	–	t	t	t	t	t	–	0.01	t	0.14	0.02	–	0.01	t	–
eucarvone	C	1245	–	0.02	0.01	0.06	0.02	–	–	0.06	–	0.02	–	–	0.01	0.14	0.24	0.05	0.01	0.02	0.01	t
trans-2,8-*p*-mentha-dien-1-ol	B	1246	t	–	–	–	–	–	–	t	0.14	–	0.05	–	–	–	–	t	–	–	–	–
isopentyl hexanoate[e]	A	1250	0.06	t	–	t	t	–	t	–	–	–	–	0.03	–	–	–	–	–	t	t	–
p-anisaldehyde[e]	A	1251	t	t	t	–	t	–	–	0.02	–	t	–	–	0.01	–	t	t	–	t	t	–
piperitone[e]	B	1251	–	t	t	–	t	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
carvenone[e]	B	1252	–	–	0.01	–	–	–	–	–	t	–	–	–	–	–	–	–	–	–	–	–
2,6,6-trimethyl-1-cyclo-hexene-1-acetaldehyde[e]	C	1254	t	–	t	t	t	–	–	t	–	t	–	–	–	–	–	t	–	–	–	t
geraniol	A	1255	t	–	t	–	–	–	–	–	–	–	t	–	–	–	–	–	t	–	–	–
2-phenylethyl acetate[e]	A	1256	t	t	t	t	t	–	t	t	–	–	–	–	0.01	–	–	t	–	–	–	–
benzyl propanoate[e]	A	1257	t	t	t	t	–	–	–	–	–	–	–	–	0.01	–	–	t	0.01	–	t	–
γ-octalactone	A	1260	0.06	0.01	t	t	0.03	–	–	0.07	0.09	0.03	–	–	–	0.07	0.10	0.04	t	0.04	0.02	0.02
(*E*)-2-decenal	A	1261	–	t	0.01	–	–	–	–	–	–	–	–	–	0.01	0.04	t	0.01	0.01	t	t	–

Table 1. (Continued)

compound	ID[b]	RI[c]	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
(*E*)-cinnamaldehyde[e]	B	1266	t	–	t	–	–	–	–	–	–	t	–	–	0.03	t	t	t	–	–	t	–
ethyl salicylate[e]	A	1267	0.01	0.02	0.04	t	0.01	–	t	0.03	t	t	t	t	t	t	0.02	0.01	t	0.01	0.01	–
geranial	B	1270	0.04	0.02	0.04	0.03	0.04	–	t	0.03	t	0.06	0.01	t	0.05	0.05	0.06	0.03	0.01	0.03	0.03	–
citronellyl formate[e]	A	1275	t	t	0.01	t	t	–	t	–	–	–	–	t	0.01	t	0.01	t	0	t	t	–
nonanoic acid	A	1280	0.03	t	0.01	t	t	–	t	–	–	0.53	t	–	t	t	t	t	0.19	t	t	0.09
α-terpinen-7-al[e]	B	1282	t	t	0.02	t	–	–	–	0.02	–	t	–	–	–	t	0.08	–	t	–	–	0.01
(*E*)-anethole[e]	A	1283	0.12	t	0.07	t	0.04	–	t	0.06	–	0.09	t	–	0.14	t	0.08	0.10	–	–	t	0.02
bornyl acetate[e]	A	1285	t	t	0.07	0.05	0.04	t	0.03	t	0.05	t	0.10	0.04	t	0.15	t	t	–	0.08	0.08	–
safrole	A	1287	t	t	t	t	–	–	t	0.02	–	–	t	–	t	t	t	t	–	t	t	–
diallyl trisulfide[e]	C	1289	0.02	0.01	t	t	–	–	t	0.02	–	t	t	–	0.02	t	0.03	0.02	–	t	0.01	–
thymol	A	1290	t	0.02	0.12	t	t	–	t	t	t	t	0.03	t	0.04	0.03	0.01	0.01	t	t	0.01	–
ethyl nonanoate[e]	A	1294	0.04	0.05	t	t	0.03	0.13	0.02	0.04	–	0.15	0.05	t	0.03	0.08	0.04	0.02	0.02	0.02	0.01	0.05
carvacrol	A	1298	t	t	0.01	t	t	–	t	t	–	t	–	–	0.01	t	t	t	0.01	t	t	t
undecanal[e]	A	1306	–	–	–	–	–	–	–	–	–	0.04	–	–	–	–	–	–	–	–	–	–
4-vinylguaiacol[e]	A	1312	t	t	0.01	t	t	–	–	–	–	t	–	–	t	–	–	t	–	–	–	–
4-propylanisole[e]	A	1319	t	–	0.01	–	t	–	–	–	–	t	–	–	0.01	–	–	–	t	–	t	–
methyl decanoate[e]	A	1326	t	0.01	t	t	t	–	–	–	–	t	t	–	t	t	t	0.01	0.02	0.01	–	–
allyl phenylacetate[e]	A	1328	0.02	0.04	0.07	–	t	–	t	–	–	t	–	–	0.04	0.01	0.04	0.01	t	t	0.01	–
piperonal[e]	A	1329	t	t	t	–	t	–	–	–	–	t	–	–	t	–	t	–	–	–	t	–
trans-carvyl acetate	B	1337	–	–	t	t	–	–	–	–	–	t	–	–	–	–	–	–	–	–	–	–
methyl anthranilate[e]	A	1338	t	0.01	0.03	t	t	–	–	0.01	–	0.02	t	–	0.02	0.01	0.01	0.01	–	t	0.01	–
4-acetylanisole[e]	A	1345	0.02	–	–	–	–	–	–	0.16	–	–	–	–	–	0.01	–	–	–	–	–	–
benzyl butanoate[e]	A	1347	t	t	t	t	t	–	–	–	–	t	t	–	0.01	0.02	0.01	0.01	–	t	0.01	–
dehydroionene[e]	C	1348	0.02	0.02	0.03	t	t	–	t	t	–	0.03	t	–	0.01	t	–	t	0.01	–	t	–
α-terpinyl acetate	A	1350	t	t	t	–	–	–	t	–	–	t	t	–	t	t	t	t	–	–	–	–
citronellyl acetate	A	1354	–	–	t	t	–	–	–	–	–	–	–	–	–	–	t	t	–	–	–	–
eugenol	A	1356	t	t	0.01	t	t	–	–	–	t	t	t	–	0.01	t	t	t	t	t	t	–
benzyl isothiocyanate[e]	A	1359	t	t	t	–	t	–	–	–	–	t	t	–	t	t	t	t	–	t	t	–
γ-nonalactone	A	1360	t	0.01	0.02	t	t	–	–	–	–	t	t	–	0.01	t	t	0.01	t	t	0.01	t
neryl acetate	A	1365	0.02	t	0.01	0.01	t	–	0.01	t	t	t	t	t	0.01	0.02	0.02	0.01	0.01	0.01	0.01	t
α-copaene	B	1376	0.03	0.02	t	0.01	t	t	0.03	0.01	t	0.05	t	0.12	0.02	0.06	0.02	0.02	0.09	0.01	0.01	t
butyl benzoate[e]	A	1377	t	t	0.03	t	–	–	–	–	–	t	t	–	–	t	–	t	t	t	t	t
2-butyl-2-octenal[e]	C	1378	t	t	t	t	t	–	–	t	–	t	t	–	0.01	0.01	0.02	0.01	–	t	0.01	–
methyl (*E*)-cinnamate[e]	A	1379	t	t	t	t	t	–	–	t	–	t	–	–	t	0.01	0.01	t	–	t	t	t
decanoic acid	A	1380	t	t	t	t	t	–	–	t	–	t	–	–	–	t	–	0.01	–	–	–	t
(*E*)-β-damascenone	B	1381	0.03	0.01	0.08	t	t	–	t	–	0.05	0.06	0.01	0.01	0.04	t	0.01	0.02	0.05	0.01	0.03	0.02
geranyl acetate	A	1383	0.03	t	0.02	t	t	–	0.01	0.02	t	0.04	t	–	0.03	0.02	0.03	0.03	t	t	0.02	t
hexyl hexanoate	A	1385	–	–	–	–	–	–	–	–	–	–	–	t	–	–	–	–	–	–	–	–
β-elemene	B	1391	t	0.02	–	0.02	t	–	–	t	0.04	–	–	–	t	0.04	t	t	0.07	0.01	–	0.01
isobutyl phenylacetate[e]	A	1392	t	t	0.01	–	t	–	–	–	–	t	–	–	t	t	–	t	–	–	–	–
butyl octanoate[e]	C	1393	t	–	–	0.02	–	–	–	–	–	–	–	–	–	t	–	t	–	–	–	–
octyl isobutanoate[e]	A	1394	–	–	–	–	–	–	–	–	t	–	–	–	–	–	–	–	–	–	–	–
benzyl isopentanoate[e]	A	1395	0.02	0.02	0.06	0.02	t	–	0.01	0.02	t	0.03	0.02	t	0.04	0.04	0.05	0.03	0.01	0.01	0.02	–
diphenyl ether[e]	A	1396	t	t	t	t	t	–	t	t	t	t	t	t	t	t	t	t	t	t	t	t
ethyl decanoate	A	1397	0.03	0.02	t	0.10	t	–	t	0.01	0.29	0.01	0.01	0.16	0.02	0.16	0.08	0.19	t	0.05	t	–
methyl *N*-methyl-anthranilate[e]	B	1402	t	t	0.04	–	–	–	t	–	–	t	t	–	–	–	–	–	–	t	–	–
α-gurjunene	B	1407	–	–	t	0.18	0.11	–	–	0.24	0.88	0.05	–	–	0.25	0.19	–	0.15	0.07	–	–	0.01
α-cedrene[e]	B	1409	0.07	0.03	0.04	t	t	0.18	0.04	t	t	t	0.01	0.05	t	t	0.18	–	–	0.09	0.08	–
methyleugenol[e]	A	1410	t	t	t	–	t	–	t	–	–	t	t	–	t	–	–	t	t	–	–	–
β-caryophyllene	A	1418	0.07	0.16	0.68	0.59	0.41	0.71	0.08	1.35	4.65	0.28	t	0.18	1.48	0.75	1.04	1.24	0.61	1.28	0.88	0.14
allyl cyclohexylpro-panoate[e]	A	1420	0.01	0.01	0.02	t	0.01	–	–	–	–	t	t	–	0.01	t	t	0.02	t	t	0.02	–
α-(*E*)-ionone[e]	A	1426	t	t	0.01	t	–	–	t	–	–	t	t	–	t	t	t	t	–	t	–	t
methyl undecanoate[e]	A	1427	0.02	t	0.01	t	0.01	–	0.01	0.01	t	0.01	t	t	0.02	0.02	0.03	0.02	t	0.01	0.01	t
α-*trans*-bergamotene	B	1436	0.02	t	0.01	0.03	0.01	t	t	0.05	t	0.01	t	t	0.02	0.02	0.04	0.02	0.01	0.02	0.02	t
α-guaiene	B	1439	–	–	–	–	t	t	0.04	–	–	–	–	0.10	t	–	–	–	–	–	–	–
2-phenylethyl butanoate	A	1440	0.01	t	0.01	t	t	–	t	0.01	–	0.01	t	–	0.01	t	0.01	0.04	0.01	0.04	0.01	t
benzyl pentanoate[e]	C	1445	0.04	t	t	–	t	–	–	–	–	–	t	–	t	–	t	–	–	–	t	–
geranylacetone	A	1453	t	0.01	0.11	0.02	0.01	–	–	0.08	–	0.02	t	t	0.04	0.04	t	t	0.02	0.01	0.01	0.10
α-humulene	A	1454	t	0.10	0.47	0.39	0.27	0.40	0.05	0.86	3.07	0.18	t	0.13	0.89	0.51	0.65	0.79	0.37	0.78	0.58	0.08
9-*epi*-(*E*)-caryophyllene[d]	B	1465	t	t	–	t	t	–	–	t	–	t	–	–	–	t	0.01	0.01	t	t	t	–
ethyl (*E*)-cinnamate[e]	A	1467	t	0.01	t	t	t	–	–	–	–	t	–	–	t	0.01	t	0.01	0.01	–	t	0.02
drima-7,9(11)-diene	B	1469	0.02	–	–	0.21	0.13	0.08	t	0.13	0.21	–	–	–	–	–	t	t	–	0.05	t	–
γ-decalactone	A	1470	0.02	0.02	0.02	t	t	–	–	0.03	–	t	t	–	0.02	0.04	0.07	0.03	t	0.04	t	t
γ-gurjunene	B	1472	–	–	–	t	t	–	–	–	0.04	–	–	t	t	–	–	–	–	–	–	t
β-chamigrene	B	1475	t	t	–	t	t	–	–	t	–	t	–	t	–	–	–	–	–	–	t	–
selina-4,11-diene[e]	B	1476	–	0.02	t	0.04	0.03	–	–	–	t		–	–	0.01	t	0.01	t	0.05	–	–	–
γ-muurolene	B	1477	t	t	0.01	t	t	–	0.01	0.01	0.09	t	–	t	t	t	0.06	t	0.06	t	0.01	0.01
geranyl propanoate[e]	A	1478	t	t	t	t	–	–	t	t	–	–	t	–	0.01	t	t	0.01	–	–	–	–
germacrene D	B	1480	0.02	t	0.02	–	0.02	–	0.05	t	t	–	t	0.20	0.01	0.13	–	–	t	–	–	–
β-selinene	B	1484	t	t	t	t	t	–	0.02	t	t	t	t	0.02	–	0.09	–	t	t	0.01	t	0.11
eremophilene	B	1486	0.11	t	–	2.08	t	0.99	t	1.06	2.10	0.07	0.03	t	–	–	t	–	0.03	0.27	0.09	–
ar-curcumene[e]	B	1487	t	t	t	–	–	–	t	–	–	t	t	t	t	t	t	0.02	t	–	–	–

Table 1. (Continued)

compound	ID[b]	RI[c]	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
(*E*)-β-ionone	A	1488	0.04	0.03	0.14	0.07	0.09	0.04	0.02	0.26	0.09	0.11	0.01	0.04	0.07	0.12	0.02	0.03	0.02	0.03	0.02	0.02
valencene	A	1491	0.02	–	–	0.20	0.14	–	t	0.12	0.29	t	t	–	–	t	t	–	t	t	t	–
α-selinene	B	1493	0.02	0.01	0.02	0.20	0.14	0.28	0.03	0.12	0.29	0.02	t	0.08	0.05	0.16	0.04	0.04	0.06	–	0.03	t
α-zingiberene[e]	B	1495	0.01	t	t	t	t	t	0.03	t	–	t	–	–	t	0.01	t	t	–	0.03	0.01	–
δ-decalactone	A	1496	t	0.01	t	–	–	–	–	t	–	t	–	–	–	0.01	0.02	–	0.01	0.03	t	–
viridiflorene[e]	B	1497	t	0.01	0.02	0.06	0.05	–	t	0.05	0.10	–	–	–	0.01	–	–	t	0.08	0.02	t	t
ethyl undecanoate[e]	A	1498	t	–	0	–	–	–	–	–	–	–	–	–	t	–	–	t	–	–	–	–
(*E*)-methylisoeugenol[e]	A	1500	–	t	t	–	t	–	t	–	–	t	–	–	–	t	–	–	–	–	–	–
α-bulnesene	B	1505	–	–	0.01	t	t	–	0.08	t	t	–	–	0.27	t	–	–	–	–	t	t	–
β-bisabolene[e]	B	1509	0.06	0.03	0.02	0.02	0.02	–	0.02	0.05	0.02	0.01	t	0.04	0.03	0.08	0.07	0.04	t	0.02	0.02	t
tridecanal[e]	A	1511	–	–	0.02	–	–	–	–	–	–	0.08	–	–	–	–	–	–	–	–	–	0.12
7-*epi*-α-selinene	B	1517	t	–	–	0.09	0.06	0.06	t	0.06	0.12	t	t	t	–	–	–	–	–	0.03	0.02	–
2-methyl-β-ionone[e]	B	1519	t	t	0.02	t	t	–	t	0.03	0.04	t	t	t	0.02	t	0.01	0.01	0.02	0.01	0.02	t
cis-calamenene[e]	B	1521	t	t	t	t	t	–	t	t	t	t	–	t	–	t	t	t	t	–	t	–
δ-cadinene		1523	0.02	0.01	0.04	0.02	0.03	t	0.04	0.03	0.08	0.02	t	0.10	0.02	0.08	0.03	0.02	0.05	0.02	0.01	0.01
β-sesquiphellandrene[e]	B	1524	t	t	–	t	t	–	–	t	–	t	–	–	t	t	t	t	t	t	0.01	t
dihydroactinidiolide	B	1525	–	t	t	t	t	–	–	t	–	t	–	–	t	–	–	–	t	t	–	t
methyl dodecanoate	A	1526	t	t	t	t	–	–	–	0.02	t	t	t	–	–	t	0.01	0.02	t	t	t	t
cadina-1,4-diene	B	1532	–	–	t	–	t	–	t	–	–	–	–	0.02	–	0.01	–	t	0.02	t	t	–
α-cadinene[e]	B	1538	–	–	t	–	t	–	–	–	–	–	t	t	t	t	–	–	0.01	–	–	–
α-calacorene[e]	B	1542	0.02	t	t	t	0.01	–	–	t	t	–	–	t	–	t	t	t	t	–	0.01	–
3,4-dihydro-8-hydroxy-3-methyliso-coumarin[e]	C	1549	t	t	0.13	t	t	–	t	t	t	t	–	–	0.01	t	–	t	–	t	t	t
germacrene B[e]	B	1556	t	–	t	–	0.01	–	t	t	t	–	–	t	t	t	0.01	t	0.01	t	t	–
caryophyllene alcohol[e]	B	1564	0	0.01	0.05	t	t	–	t	t	t	0.01	t	–	0.06	t	0.01	0.01	0.02	0.01	0.02	t
(*E*)-nerolidol[e]	A	1568	0.01	–	t	t	t	–	–	0.01	–	t	t	–	t	0.07	t	t	t	t	–	–
γ-undecalactone	A	1573	0.04	0.03	0.04	t	t	–	–	–	–	t	t	–	0.02	t	t	0.12	t	t	0.03	–
dodecanoic acid	A	1580	0.04	t	0.16	t	t	–	–	–	–	1.28	0.03	t	0.03	t	0.03	0.18	0.43	–	–	0.06
caryophyllene oxide	A	1581	t	–	t	0.02	0.04	–	–	0.14	0.08	t	–	t	0.03	0.11	0.03	t	0.02	0.07	t	–
2-phenylethyl tiglate[e]	A	1584	–	–	–	–	–	–	–	t	–	–	–	–	–	–	t	t	–	0.02	t	t
butyl decanoate[e]	C	1588	t	0.03	–	0.04	t	–	–	–	–	t	–	–	–	0.04	–	0.03	–	–	–	–
decyl isobutanoate[e]	C	1590	–	–	–	–	–	–	–	–	t	–	–	–	–	–	–	–	–	–	–	–
humulene epoxide I	B	1593	–	–	t	–	–	–	–	0.02	t	–	–	–	–	–	–	–	–	–	t	–
guaiol	B	1595	–	–	0.09	–	–	–	–	–	–	–	–	0.01	–	–	–	–	–	–	–	–
ethyl dodecanoate	A	1597	0.25	0.12	t	0.49	0.03	0.44	0.01	0.19	0.96	0.07	0.08	t	0.07	0.73	0.28	1.18	t	0.44	0.01	0.02
humulene epoxide II	B	1606	–	t	0.02	–	t	–	–	0.03	t	t	–	–	–	t	–	t	–	t	0.01	–
tetradecanal	A	1611	–	–	t	–	–	–	–	t	–	0.02	–	–	–	0.03	0.01	t	0.02	t	–	0.03
benzophenone[e]	A	1621	t	t	0.01	t	0.01	–	–	t	–	–	–	–	0.01	–	t	0.01	t	t	–	–
dill apiole	B	1622	t	t	0.03	t	t	–	0.01	t	–	–	–	–	0.01	0.01	0.01	0.01	t	t	0.02	–
γ-eudesmol[e]	B	1629	–	–	–	–	–	–	–	–	–	–	–	–	t	–	–	–	t	–	–	–
methyl tridecanoate[e]	A	1631	–	t	t	–	–	–	0.01	–	–	–	–	–	–	–	–	t	–	–	–	–
τ-muurolol[e]	B	1641	t	t	t	t	0.01	–	0.01	0.03	0.04	–	t	–	–	t	–	–	t	–	–	t
cubenol[e]	B	1642	t	t	0.07	t	t	–	t	–	0.04	t	t	t	t	t	t	–	0.02	–	–	t
α-muurolol[e]	B	1643	0.01	t	t	–	0.01	–	–	–	–	–	–	t	t	0.02	–	–	0.01	–	–	–
(*Z*)-jasminaldehyde[e]	A	1645	–	t	0.01	–	–	–	–	–	–	–	–	–	t	t	–	–	–	–	–	t
selin-11-en-4-α-ol	B	1652	0.02	0.03	t	0.06	0.07	–	0.02	t	0.10	0.01	–	0.06	0.02	0.05	0.02	0.01	0.17	t	0.01	t
α-cadinol	B	1653	t	t	0.02	–	t	–	t	t	t	–	t	–	t	t	–	–	t	–	–	–
ar-turmerone[e]	B	1664	t	t	t	t	t	–	–	0.01	–	t	t	–	t	t	–	–	–	–	–	–
bulnesol	B	1666	–	–	–	–	–	–	–	–	–	–	–	0.01	–	–	–	–	–	–	–	–
(*Z*)-3-hexenyl salicylate[e]	A	1670	t	–	–	–	–	–	–	–	–	–	–	–	–	–	t	–	–	–	–	–
cadalene[e]	B	1673	t	t	t	t	t	–	t	t	–	t	–	t	–	t	t	t	–	t	t	t
γ-dodecalactone	A	1675	t	0.01	0.02	t	t	–	–	0.02	–	0.01	t	–	t	0.01	0.02	0.01	0.27	t	t	–
tridecanoic acid[e]	A	1678	–	–	–	t	–	0.04	t	–	t	t	t	t	–	t	–	–	t	–	–	t
propyl dodecanoate[e]	C	1685	0.02	0.01	–	0.01	–	–	–	–	t	–	–	–	–	–	t	–	–	–	–	–
(*Z*)-11-pentadecenal[e]	C	1686	t	t	0.04	t	t	–	–	0.38	–	0.19	–	–	–	0.66	0.41	0.14	0.06	0.14	0.01	1.65
ethyl tridecanoate[e]	A	1687	t	t	–	t	t	–	–	–	–	–	–	–	–	t	–	t	–	–	–	–
2-pentadecanone[e]	A	1689	t	–	0.01	t	t	–	–	0.01	–	0.01	–	t	t	–	0.01	t	0.03	–	–	–
pentadecanal[e]	C	1711	0.04	t	0.11	0.04	t	0.44	–	0.27	–	0.40	–	–	–	0.94	0.48	0.17	0.13	0.34	0.02	2.44
(*Z*,*Z*)-farnesol[e]	B	1713	t	–	0.02	–	–	–	–	–	–	t	–	–	t	–	–	–	–	t	t	t
methyl tetradecanoate[e]	A	1726	0.01	0.01	t	t	–	–	–	0.11	t	t	–	–	t	t	0.01	0.06	0.02	0.01	t	t
(*E*,*Z*)-farnesol[e]	B	1742	t	t	t	t	–	–	–	–	–	t	–	–	–	t	–	t	–	–	–	t
isobutyl dodecanoate[e]	C	1753	t	–	–	t	–	–	–	t	–	–	–	–	–	–	–	–	–	0.01	–	t
benzyl benzoate[e]	A	1762	0.02	0.01	t	0.02	–	–	–	–	–	–	–	–	0.01	–	0.09	t	0.02	0.02	0.02	t
tetradecanoic acid	A	1780	0.73	0.28	1.33	0.21	1.09	–	0.04	0.85	t	1.62	1.36	0.08	0.56	0.79	0.16	0.83	1.00	0.47	0.03	1.51
(*Z*)-9-tetradecenoic acid[e]	A	1783	–	–	–	–	t	–	–	0.16	–	–	–	–	–	–	0.02	t	–	–	–	–
butyl dodecanoate[e]	C	1786	0.05	–	–	0.11	–	–	–	t	t	–	–	–	–	0.08	0.01	0.09	–	0.92	–	–
ethyl tetradecanoate	A	1793	0.73	0.29	–	0.74	0.26	0.84	0.03	0.74	2.27	0.44	0.18	0.22	0.12	t	0.84	3.90	0.34	t	0.09	0.40
hexadecanal[e]	C	1811	0.11	0.19	–	t	0.14	–	t	0.14	0.06	–	–	t	0.22	0.54	0.05	0.52	t	0.05	0.01	t
benzyl salicylate[e]	A	1863	t	t	–	t	t	–	–	–	–	–	–	t	t	–	0.06	t	t	0.03	–	–
pentadecanoic acid[e]	A	1878	0.03	t	t	t	0.09	–	t	0.04	–	0.13	t	t	–	–	0.01	t	t	t	0.02	0.21
1-hexadecanol	A	1879	0.88	1.31	0.06	0.15	1.14	–	0.01	0.76	0.59	0.03	0.03	0.01	0.99	1.87	0.15	2.25	0.11	0.12	0.07	–

Table 1. (Continued)

compound	ID[b]	RI[c]	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
methyl linolenate	A	1893	0.02	0.03	–	0.05	–	–	–	0.36	–	–	–	–	–	0.37	0.29	–	–	0.63	t	–
propyl tetradecanoate[e]	A	1896	0.02	t	–	0.05	–	–	–	–	–	–	–	–	0.02	–	–	0.34	–	–	–	–
ethyl pentadecanoate[e]	A	1897	0.02	t	–	t	t	–	–	t	t	–	–	–	–	t	t	0.05	–	t	t	t
2-heptadecanone[e]	C	1900	–	t	t	–	–	–	–	–	–	–	t	t	t	t	–	t	t	t	–	–
(*E*,*E*)-farnesyl acetone[e]	B	1921	0.08	t	0.27	0.04	0.07	–	–	0.28	–	t	–	–	0.04	0.09	–	–	0.18	t	0.05	0.21
methyl hexadecanoate[e]	A	1926	0.02	0.01	0.03	0.02	0.01	–	–	t	0.13	0.01	t	t	0.01	0.03	0.06	0.09	0.22	0.03	t	0.06
methyl palmitoleate[e]	A	1932	t	t	t	t	t	t	t	t	t	–	–	–	–	–	t	t	–	t	t	–
(*Z*)-9-hexadecenoic acid	C	1953	t	t	t	t	–	–	–	t	0.74	0.25	t	t	t	t	0.16	t	–	0.02	–	–
butyl tetradecanoate[e]	C	1986	t	–	–	t	–	–	–	–	–	–	–	–	–	–	–	t	–	–	–	–
ethyl (*Z*)-9-hexadecenoate	C	1990	2.13	1.96	t	2.52	2.81	–	0.18	2.58	2.16	t	2.99	0.26	0.82	1.05	0.57	1.97	t	1.05	0.52	1.57
hexadecanoic acid	A	1991	1.18	1.44	1.59	1.09	1.92	0.24	0.59	1.59	1.23	1.58	1.21	0.63	1.06	1.76	1.54	1.63	1.73	1.07	0.46	1.44
ethyl hexadecanoate	A	1.993	2.54	1.39	t	1.10	2.08	t	0.17	1.07	1.89	–	0.46	0.11	2.61	2.72	2.61	2.01	2.40	2.19	0.36	0.67
isopropyl hexadecanoate[e]	C	1999	0.37	0.26	–	–	0.45	–	–	–	–	–	–	–	–	–	–	–	–	t	t	–
propyl hexadecanoate[e]	C	2091	0.15	0.07	–	t	0.03	–	–	0.18	0.34	t	–	t	0.01	0.12	0.07	0.09	–	0.03	–	–
methyl linoleate[e]	A	2093	0.09	0.03	t	t	0.02	–	–	0.22	–	–	–	–	–	–	–	t	–	–	–	–
methyl oleate[e]	A	2103	–	–	–	0.03	–	–	–	0.16	0.10	t	t	–	t	t	t	–	–	t	–	–
methyl octadecanoate[e]	A	2128	–	0.10	–	–	–	–	–	–	–	–	–	–	–	–	t	t	0.74	–	–	0.09
isobutyl hexadecanoate[e]	C	2135	–	–	–	–	–	–	–	0.84	–	–	–	–	–	–	t	–	t	–	–	0.49
oleic acid	A	2141	–	t	–	t	t	–	–	t	–	0.57	–	–	–	0.67	t	0.76	–	t	0.86	–
ethyl linoleate	A	2159	2.72	0.12	–	0.33	t	–	–	0.29	1.52	–	1.83	0.02	–	0.28	t	0.11	–	0.09	0.17	t
ethyl linolenate	A	2169	t	–	t	1.21	t	–	0.19	0.69	3.01	t	0.33	0.20	t	0.60	–	0.45	–	0.46	t	–
octadecanoic acid	A	2172	t	–	–	t	–	–	t	–	–	0.79	–	–	–	–	–	–	1.35	–	t	1.44
ethyl oleate	A	2179	0.67	–	1.09	0.38	t	–	0.03	0.14	1.48	–	0.19	t	t	0.31	0.08	t	–	0.16	0.19	–
butyl hexadecanoate[e]	C	2188	0.28	–	–	0.09	–	–	t	–	0.40	–	–	–	t	0.15	0.05	0.22	–	t	0.09	t
ethyl octadecanoate[e]	A	2193	0.70	0.19	t	0.08	t	0.05	0.03	0.21	0.79	0.08	0.06	t	t	0.22	0.09	0.20	t	0.09	0.13	0.53
isopentyl hexadecanoate[e]	C	2260	t	–	–	–	–	–	–	–	t	–	–	–	t	–	–	t	–	–	–	–
propyl octadecanoate[e]	C	2296	0.01	t	–	t	–	–	–	–	–	–	–	–	–	–	–	t	–	–	–	–
butyl octadecanoate[e]	C	2388	0.11	0.15	–	t	t	–	–	–	–	–	–	–	–	–	–	t	–	–	–	–
total volatiles (ppm)			33.97	27.42	20.31	45.79	47.80	35.52	23.62	64.40	122.46	27.33	17.62	38.67	26.02	59.68	59.92	42.06	19.57	30.78	28.24	25.19

[a] 1, cv. Delicioso; 2, cv. Haden; 3, cv. Super Haden; 4, cv. Manga amarilla; 5, cv. Macho; 6, cv. Manga blanca; 7, cv. Ordoñez; 8, cv. Obispo; 9, cv. Corazón; 10, cv. Delicia; 11, cv. Filipino; 12, cv. Huevo de toro; 13, cv. San Diego; 14, cv. Manzano; 15, cv. Smith; 16, cv. Florida; 17, cv. Minin; 18, cv. La Paz; 19, cv. Keitt; 20, cv. Kent. [b] The reliability of the identification proposal is indicated by the following: A, mass spectrum and Kovats index agreed with standards; B, mass spectrum and Kovats index agreed with literature data; C, mass spectrum agreed with mass spectral database. [c] Retention index on HP-5MS. [d] t, <0.01 mg/kg. [e] Reported for the first time in mango. [f] –, not detected.

A number of significant differences can be observed on the basis of the quantitative distributions of terpene hydrocarbons in the studied cultivars. The terpene δ-3-carene was the dominant compound in 10 cultivars: Haden, Manga amarilla, Macho, Manga blanca, San Diego, Manzano, Smith, Florida, Keitt, and Kent. Five of the studied cultivars were rich in limonene: Delicioso, Super Haden, Ordoñez, Filipino, and La Paz, whereas cv. Delicia was rich in both δ-3-carene and limonene. Terpinolene was present in a considerable amount in three other cultivars: Obispo, Corazón, and Huevo de toro. Only one cultivar, Minin, was rich in α-phellandrene. In previous studies, the terpene δ-3-carene was the dominant compound of a Venezuelan cultivar (*28*), Tommy Atkins and Keitt cultivars from Florida (*11*), Tommy Atkins from Australia (*5*), Corazón, Bizcochuelo, and Super Haden cultivars (*13*), M'Bingue, Téte de Chat, and Palmer cultivars grown in Africa (*6*), Haden, Rubi, and Tommy Atkins cultivars (*14*), and Haden, Tommy Atkins, and Keitt cultivars (*16*). Limonene was the major contributor to Baladi (*6*) and was present in considerable amounts in Carlota and Bacuri cultivars (*16*). The compound terpinolene occurred in considerable quantity in Willard and Parrot cultivars from Sri Lanka (*10*), in Bowen (*17*), Kensington Pride, and Florigon cultivars grown in Australia (*12*), and in Espada (*14*). Myrcene was the major contributor in Alphonso (*8*) and in Mapulevu (*12*). The terpenes (*Z*)- and (*E*)-β-ocimene were found in considerable amounts in Alphonso cultivar grown in India (*27*), and (*Z*)-β-ocimene was found in high amounts in Jaffna mango from Sri Lanka (*10*) and Amélie cultivar from Africa (*6*).

The hydrocarbons (*Z*)- and (*E*)-β-ocimene have a warm, herbaceous, and floral odor, whereas the odor of δ-3-carene was sweet, reminiscent of refined limonene (*38*). Myrcene and (*Z*)-β-ocimene were reported to be responsible for the green aroma of raw mangos (*39*). The compound δ-3-carene was considered to be the major aroma-contributing component in some mangos (*11*, *28*), whereas the green aroma note typical of mango was correlated to monoterpene hydrocabons (*14*). Taking into account the strong and characteristic aromas of monoterpene hydrocarbons, the simple differences partly explain the known differences in flavor among the Cuban cultivars.

Among the sesquiterpene hydrocarbons, β-caryophyllene, α-humulene, and eremophilene were found to predominate in almost all Cuban cultivars. The first two compounds have also been found in significant quantities in other mangos (*8*, *10*, *14*, *27*). Eremophilene, the principal volatile compound ascribed to the African mango (*40*), was also found in some studied cultivars, whereas it could not be found in Brazilian fruits (*16*). The compound β-selinene, which was detected in considerable amount in Venezuelan fruit (*28*), in Willard and Parrot cultivars (*10*), and in African cultivars (*6*), was found in significant amount in only the Kent mango.

The next class in importance after the terpene hydrocarbons was that of the esters, totaling 90 aliphatic, 16 aromatic, and 8 terpene esters found in the studied cultivars. Among them, ethyl acetate and ethyl butanoate were the major ones. Large amounts of ethyl butanoate were observed in Baladi mango from Egypt (*8*), Kensington Pride grown in Australia (*17*), and Cuban cultivars (*13*). Ethyl butanoate was reported to be responsible for the fruity flavor of mango (*14*). Esters, especially straight-chain esters, are generally metabolized from fatty acids through β-oxidation (*41*). Biosynthesis of fatty acids, the precursors of esters, has been found to be high during ripening of mango (*19*). In addition to several straight-chain esters, many esters of branched-chain acids were detected. These compounds comprise saturated and unsaturated esters with 2-methylpropanoate, 2-methylbutanoate, methacrylate, and tiglate residues. They can be derived from amino acid metabolism. Other detected esters of unsaturated acids were ethyl (*Z*)-3-hexenoate and butyl (*E*)-2-butenoate. The first one possesses a strong fruity aroma with a pineapple-like note (*42*), whereas (*E*)-2-butenoic acid esters had a characteristic aroma of green mango (*9*). Among the esters detected were several terpene esters (acetates of citronellol, *trans*-carveol, α-terpineol, nerol, geraniol, and borneol), besides citronellyl formate and geranyl propanoate identified for the first time in mango. A very wide range of esters of benzyl alcohol, benzoic acid, and salicylic acid was detected, many of them reported for the first time in mango. Of them, methyl benzoate was the main constituent in many of the cultivars. This ester, described as having a deep-floral odor with fruity undertones (*38*), has a low odor detection threshold of 0.52 ppb (*43*). It might therefore contribute significantly to the overall aroma of the studied cultivars. Two esters of 2-aminobenzoic acid (methyl anthranilate and methyl *N*-methylanthranilate) were newly detected in mango. Methyl anthranilate has a musty−fruity and somewhat dry-floral odor (*38*) and an odor detection threshold of 3 ppb (*44*), whereas methyl *N*-methylanthranilate has a musty−floral, sweet, and rather heavy mandarin-peel-like odor (*37*). They might therefore contribute to the overall aroma of some of the analyzed cultivars.

Lactones, as intramolecular esters of 4- and 5-hydroxy acids, were also detected. They were characterized previously in mangos (*8*, *13*, *26*, *27*), and are considered to be important contributors to the flavor and aroma of this fruit (*26*, *45*). The compound γ-octalactone, which gives a sweet herbaceous, coconut-like odor and taste (*38*), was found to be the major one and to occur above its odor detection threshold of 7 ppb (*46*) in some of the analyzed cultivars, so it might contribute to the overall aroma of the ripe fruit. In addition to lactones, we could identify esters of 3-hydroxybutanoic and 3-hydroxyhexanoic acid. Ethyl esters of these hydroxy acids have been found in a previous study of mango (*8*), but methyl 3-hydroxybutanoate is reported for the first time in mango. Its odor detection threshold does not appear to have been reported.

Among 79 identified carbonyls, only 9 of them, that is, hexanal, (*E*)-2-hexenal, (*E*,*Z*)-2,6-nonadienal, (*E*)-2-nonenal, (*Z*)-11-pentadecenal, pentadecanal, hexadecanal, 2,5-dimethyl-4-methoxy-3(2*H*)-furanone, and (*E*)-β-ionone, were found in quantifiable amounts in some cultivars. All of them except the last two are produced via lipid metabolism (*47*). Hexanal and (*E*)-2-hexenal possessed fatty-green, grassy odor and green-fruity, fresh-green odor, respectively, and both might contribute to this aroma quality of Macho and Obispo cultivars. The melon-like flavor of many studied cultivars should be related to (*E*,*Z*)-2,6-nonadienal and (*E*)-2-nonenal (*8*), known to contribute to the aroma of cucumbers (*48*). Their low odor detection thresholds of 0.1 and 0.5−1.0 ppb (*48*), respectively, suggest that they might be important contributors to the overall aroma of mango fruits.

Contrary to other reports on mango (*26*, *28*), 2-furfural and 5-methyl-2-furfural, known to be thermal degradation products of carbohydrates, were found to be absent or found in minor amounts. The compound 2,5-dimethyl-4-methoxy-3(2*H*)-furanone, commonly named mesifuran and previously reported in mango fruits (*6*, *8*, *26*, *27*), was present in almost all of the studied cultivars. This constituent, described as having a sherry wine-like note (*26*), has a very low odor detection threshold of 0.03 ppb (*49*). It might therefore contribute significantly to the overall aroma of some of the studied cultivars. The corresponding hydroxy compound, 2,5-dimethyl-4-hydroxy-3(2*H*)-furanone, commonly named Furaneol, which was identified as a mango volatile component (*27*, *45*), was not detected in this study. This is due to the chosen method of steam distillation to prepare the aroma extract (*8*, *27*).

The presence of (*E*)-β-ionone, a product of carotenoid oxidation (*47*), which has been described as having a violet-like aroma (*38*) with an odor detection threshold of 0.007 ppb (*50*), might be an important contributor to the overall aroma of the studied cultivars, particularly Obispo, Delicia, and Manzano cultivars.

Similar to carbonyls, two main biogenetic pathways can be considered for alcohols, that is, amino acid metabolism and lipid peroxidation pathways leading to unsaturated alcohols. Several terpene and aromatic alcohols were also detected. Of them, butanol, (*Z*)-3-hexenol, 1-hexanol, and 1-hexadecanol were present in notable amounts in many studied cultivars. These alcohols have been reported in high amounts in other studies (*7*, *8*, *16*, *27*). Except for (*Z*)-3-hexenol, which has a powerful and intensely green, grassy odor (*38*), the contribution of the other alcohols to the aroma is probably low because they generally have high odor detection thresholds.

A total of 17 acids were detected in the 20 cultivars, 4 of them [2-methylpropanoic, tridecanoic, (*Z*)-9-tetradecenoic, and pentadecanoic acid] reported for the first time in mango. Hexadecanoic acid was the major one in many cultivars. Acids probably contribute little to the aroma, because they generally have high odor detection thresholds.

In the group of S and N compounds, six constituents were identified: 1,2-benzothiazole, phenylacetonitrile, and among them the newly identified diallyl disulfide, diallyl trisulfide, benzyl isothiocyanate, and 2,5-dimethylpyrazine.

Other minor differences among components are also evident from **Table 1**, but the many mango cultivars usually have a wide range of aromas, and therefore a considerable variation in volatile compounds is expected, even in such a small sample. Because the aroma varies widely among cultivars, there is no one typical composition of volatile compounds for this fruit.

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