High-Resolution Gas Chromatography-Mass Spectrometry and -Fourier Transform Infrared Analysis of Cherimoya (Annona cherimolia, Mill.) Volatiles

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The volatiles of fresh cherimoya (Annona cherimolia, Mill.) fruit pulp were separated by standard controlled high-vacuum distillation and solvent extraction (pentane-dichloromethane mixture, 2:1). After preseparation by adsorption chromatography on silica gel using a pentane-diethyl ether gradient, the three fractions obtained were analyzed by capillary gas chromatography and combined capillary gas chromatographic techniques, i.e., on-line mass spectrometry and FTIR spectroscopy. In total, 208 volatiles could be identified by these methods. Among them, 23 hydrocarbons, 58 esters, 54 alcohols, 47 carbonyls, and 26 volatiles of miscellaneous structures were found. Quantitatively, alcohols such as 1-butanol, 3-methyl-1-butanol, 1-hexanol, and linalool and a series of butanoates and 3-methylbutyl esters comprised the major part of the volatiles. Among different terpenes, some terpene esters and various bicyclic derivatives were remarkable.

Economically, the family of Annonaceae is of appreciable importance as a source of edible fruits; pawpaw (Asimia), sweetsop, soursop, custard apple, ilama, and cherimoya, and plants of the genera Cananga and Rollinia have to be mentioned here. Recently, the phytochemistry of the Annonaceae has been reviewed by Leboeuf et al. (1982). Detailed reviews on tropical fruit flavors have been provided by Dupaigne (1978), Inglett and Charalambous (1979), Nagy and Shaw (1980), Ramteke et al. (1981), and Herrmann (1981). The fine taste and flavor of cherimoya (Annona cherimolia, Mill.) fruit is well-known (Brücher, 1977; Herrmann, 1983); however, investigations of the aroma composition of this fruit are lacking. Therefore, we studied the cherimoya fruit volatiles using the standard combination of capillary gas chromatography-mass spectroscopy (HRGC-MS). Furthermore, in this study, the on-line HRGC-FTIR technique (Erickson, 1979; Azzaraga and Potter, 1981) has been included.

EXPERIMENTAL SECTION

Fruits. Fresh cherimoya (A. cherimolia, Mill.) fruits were kindly purchased by K. Kaplaner, S. A., La Cruz, Chile.

Solvents. All solvents used were analytical-grade materials and additionally purified by distillation.

Isolation of Volatiles. After separation of the skin and the kernels, 4 kg of fresh fruit pulp was obtained from 6 kg of total fruit. One kilogram was placed into a 4-L three-neck bottle. After addition of internal standards (butylbenzene, 253 μ g; 2-thiophenecarboxaldehyde, 244 μ g; 1-undecanol, 240 μ g) the pulp was subjected to high-vacuum distillation.

High-Vacuum Distillation. An aliquot (1 kg) of the pulp was diluted with water (2 L) and high-vacuum distilled (40-50 °C/0.1 bar). Approximately 1 L of distillate was collected in two dry ice-methanol (-25 °C) and in two liquid nitrogen cooled traps. The four traps were thawed, and the contents were combined for the following solvent extraction. In total, 4 kg of fruit pulp was distilled in four batches.

Liquid-Liquid Extraction. The extraction of the combined aqueous distillates and the distillation residues with pentane-dichloromethane (2:1) was performed in several batches during 12 h (Drawert and Rapp, 1968). The extracts were dried over anhydrous sodium sulfate and carefully concentrated to approximately 1 mL by using a Vigreux column (45 °C). In an experiment without any standard addition, the extract obtained after high-vacuum distillation/solvent extraction had the appropriate, correct cherimoya fruit aroma properties.

Column Chromatography on Silica Gel. The concentrated distillation extract (1 mL) was fractionated on silica gel 60 (Merck), activity grade II, by using a pentane-diethyl ether gradient (Schreier et al., 1979). Cooled (11-13 °C) glass columns, 2.0 cm i.d. \times 30 cm, were used. The elution rate was 60 mL/h, and three fractions were obtained. Fraction I was eluted with 250 mL of pentane. Fraction II was obtained by eluting with 250 mL of diethyl ether-pentane (1:9 v/v), and fraction III was obtained by eluting with 250 mL of pure diethyl ether. None of the fractions showed the typical cherimoya flavor of the original extract. All eluates and the extract of the distillation residue were concentrated to 0.5 mL (for HRGC and HRGC-MS study) and to 0.05 mL (for HRGC-FTIR analysis, respectively.

Gas-Liquid Chromatography. A Carlo Erba Fractovap 4160 gas chromatograph with FID equipped with a J & W fused silica wide-bore CW 20 M capillary column (30 m, 0.0311-mm i.d.) was used. On-column injection with an air-cooled injection system was employed. The temperature program was 50-240 °C at 2 °C/min. The flow rates for the carrier gas were 2.5 mL/min He, for the makeup gas 30 mL/min N₂, and for the detector gases 30 mL/min H₂ and 300 mL/min air, respectively. The detector temperature was 220 °C. Volumes of 0.1 μ L were injected.

Qualitative analyses were carried out by means of GLC retention, mass spectral, and partly IR vapor-phase data of reference substances. Quantitative GLC determinations were performed by standard controlled calculations using a Hewlett-Packard 3388 A laboratory data system without consideration of distillation and extraction yields (calibration factors for all compounds, F = 1.00).

Gas-Liquid Chromatography-FTIR Spectroscopy. The detailed conditions of the HRGC-FTIR analysis have already been described elsewhere (Herres et al., 1983).

Gas-Liquid Chromatography-Mass Spectrometry. A Varian Aerograph 1400 gaschromatograph coupled by an open-split connection to a Finnigan MAT 44 mass spectrometer was used. The apparatus was equipped with a J & W fused silica wide-bore capillary column (CW 20

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Table I. Volatile Compounds Identified in Cherimoya Fruit Pulp by HRGC, HRGC-MS, and HRGC-FTIR

compound	peak no ^q	identified in	HRGC-	HRGC-
compound	peak no."	sinca ger traction		
(trichloroethene)	7	T	+	
(tetrachloroethene)	10	Ī	+	
1-phenoxybutene	37	Ĩ	+	
(benzene)	4	l T	+	
o-xylene	12	I T	+	
<i>m</i> - x ylene	16	Î	+	
<i>p</i> - x ylene	15	I	+	
ethylbenzene	14	I	+	
styrene 2.5-dimethylstyrene	25	I	+	
1,3-diethylbenzene	47	ÎI	+	
propylbenzene	22	I	+	
butylbenzene (std)	31	l	+	
<i>n</i> -cymene	28	I	+	
limonene	21	Ī	+	
<i>p</i> -menth-1-ene	17	I	+	
β -myrcene	18	I T	+	
(E)-ocimene	27	I	+	
(Z)-ocimene	24	Ī	+	
a-terpinene	20	I	+	
γ -terpinene	26	I	+	
a-thuiene	11	I	+	
esters		-		
diethyl carbonate	18	II	+	
ethyl acetate	2 14		+	
3-methylbutyl acetate	20	II	+	
3-methyl-2-butenyl acetate	36	II	+	
benzyl acetate	116	II	+	
linalyl acetate	88		+	
terpinyl acetate	112	Î	+	
butyl propanoate	21	II	+	
3-methylbutyl propanoate	25	II	+	
linalyl propanoate	100		+	
3-methylbutyl 2-hydroxypropanoate	91	II	+	
hexyl 2-methylpropanoate	45	II	+	
benzyl 2-methylpropanoate	129	II	+	
ethyl butanoate	13	II	+	
2-methylpropyl butanoate	22	ĨĨ	+	
butyl butanoate	31	II	+	+
2-butenyl butanoate	34		+	I
pentyl butanoate	40	II II	+	+
3-pentenyl butanoate	42	II	+	
(Z)-2-pentenyl butanoate	44	II	+	+
(E)-2-pentenyl butanoate	50		+	±
(Z)-3-hexenvl butanoate	65	II II	+	Ŧ
(E)-2-hexenyl butanoate	73	ĪĪ	+	
benzyl butanoate	132	II	+	+
butyl 2-butenoate	46		+	+
hexyl 2-butenoate	90	Î	+	
methyl 2-methylbutanoate	11	II	+	
hexyl 2-methylbutanoate	61 33		+	
3-methylbutyl 3-methylbutanoate	38	ÎÎ	+	+
3-methyl-3-butenyl-3-methylbutanoate	51	II	+	
pentyl 3-methylbutanoate	49 57	11 TT	+	
hexyl 3-methylbutanoate	64	II	+	+
(E)-3-hexenyl 3-methylbutanoate	69	II	+	-
(Z)-3-hexenyl 3-methylbutanoate	71	II	+	
benzyi 3-methylbutanoate hexyl pentanoate	134 81	11 TT	+ +	
ethyl 2-hydroxy-4-methylpentanoate	86	ĨĨ	+	
ethyl 4-oxopentanoate	75	III	+	
metnyi nexanoate	24	11	+	

Table I (Continued)

a a manual	$\mathbf{p}_{\mathbf{q}}$	identified in	HRGC-	HRGC-	
compound	реак по	silica gel traction	M8 -	FIIR	
esters					
3-methylbutyl hexanoate	68	11	+	+	
(E)-2-pentenyl nexanoate	95		+		
methyl octanoate	99 56		+		
methyl decanoate	97	II	+		
ethyl decanoate	107	Ĩ	+		
methyl pentadecanoate	157	II	+		
methyl octadecanoate	171	II	+		
methyl benzoate	102	II	+		
3-methylbutyl benzoate	136	II	+		
alcohols					
2-methyl-1-propanol	14		+	+	
1-butanol 3-methyl-1-butanol	19		+	+	
2-hutanol		TIT	+	т	
2-methyl-2-butanol	5	III	+		
2-methyl-3-buten-2-ol	10	III	+		
1-pentanol	30	III	+	+	
(E)-2-penten-1-ol	39	III	+		
(Z)-2-penten-1-ol	41	III	+	+	
(E)-3-penten-1-ol	29		+	+	
2-pentanol 4 ponton 9 el	16		+		
2-methyl-2-pentanol	21		+		
3-pentanol	16	III	+		
1-penten-3-ol	20		+	+	
cvclopentanol	38	III	+	, i	
1-hexanol	44	III	+	+	
2-ethyl-1-hexanol	66	III	+		
(E)-3-hexen-1-ol	46	III	+		
(Z)-3-hexen-1-ol	47	III	+	+	
(E)·2·hexen-1-ol	50	III	+	+	
1-hexen-3-ol	28		+		
1-neptanol	60 71		+		
(Z)-2-octen-1-ol	71 74		+		
1-nonanol	95		+		
3-nonanol	67		+		
1-decanol	109	III	+		
1-undecanol (std)	127	III	+		
1-dodecanol	138	III	+		
1-tridecanol	149	III	+		
1-tetradecanol	157	III	+		
1-nexadecanol	172		+		
1-nonadecanol	178		+		
henzylalcohol	125		+		
4-(methylethyl)benzyl alcohol	150		+		
2-phenylethanol	128	ĪĪĪ	+		
α-cadinol	160	III	+		
caryolan-1-ol	143	III	+		
geraniol	122	III	+		
linalool	83/70		+	+	
(Z)-linalool oxide, furanoid	55		+		
(Z)-linalool oxide, iuranoid	105		+		
(E)-linalool oxide, pyranoid	108	TIT	+		
mentha-?.?-dien-?-ol	117	III	+		
mentha-2,8-dien-1-ol	110	ĪĪ	+		
mentha-?,?-dien-?-ol	140	III	+		
menthol	88	III	+		
myrtenol	111	III	+	+	
nerol	114		+		
a-terpineol	98		+	+	
carbonyls	74	111	Ŧ		
3-hydroxy-2-butanone	33	III	+		
2-pentanone	8	II	+		
3-penten-2-one	17	III	+		
3-methylbutyl-2,4-pentadione	52	II	+		
cyclonexanone	34		+		
o,o,o-mmeinyrcycionexanone 6-methyl-5-henten-9-one	48 19/19	11 TT/TTT	+		
2-nonanone	40/40 54	II/ III II	+		
2-tridecanone	$1\overline{27}$	Ĩ	+		
3-tridecanone	124	ĪĪ	+		

Table I (Continued)

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compound	identified in pound peak no. ^a silica gel fraction		HRGC- MS ^b	HRGC- FTIR
carbonyls		· · · · · · · · · · · · · · · · · · ·	· · ···· — — — — — — — — — — — — — — —	
2-tetradecanone	138	TT	+	
2-pentadecanone	146	Ĩ	+	
3-pentadecanone	144	II	+	
2-heptadecanone	158	II	+	
3-heptadecanone	155	II	+	
2-octadecanone	165	II	+	
3-nonadecanone	168	II	+	
2-eicosanone	174	II	+	
3-heneicosanone	176	II	+	
3-methylacetophenone	118	II	+	
4-methylacetophenone	121	II	+	
propiophenone	113		+	
butyrophenone	123		+	
benzopnenone	170		+	
geranylacetone	131		+	
campior	114/100		+ +	
chrysanthenone	65	III	+	
menthone	57	III	+	
pinocamphone	77	II	+	
verbenone	97	ĪĪI	+	
2-methyltetrahydrofuran-3-one	32	III	+	
(E)-2-hexenal	28	II	÷	
(Z,E)-2,4-heptadienal	66	II	+	
(E, E)-2,4-heptadienal	72	II	+	
2-ethyloctanal	67	II	+	
dodecanal	115	II	+	
tetradecanal	140	II	÷	
pentadecanal	145	II	+	
benzaldehyde	79	II	+	
2-methylbenzaldehyde	95	11	+	
3-methylbenzaldehyde	96		+	
4-methylbenzaldehyde	101		+	
campholenealdenyde	72		+	
myrtenal fuufuunal	98		+	
2. thiophopogerboxaldebude (std)	100	111	+	
z-unophenecarboxandenyde (stu)	105	11	Ŧ	
2.6.6.trimethyl-2-vinyltetrahydronyran	19	TĪ	+	
2.0.00 miniculty 2.00 my the training at opy tail	32	Ĩ	+	
propenyl) tetrahydrofuran	02			
5-(methylethyl)-2-methyl-2-	37	II	+	
vinvltetrahydrofuran				
1.8-cineole	27	II	+	
phenol	139	III	+	
<i>m</i> -cresol	148	III	+	
thymol	158	III	+	
anethol	127	II	+	
1,4-dimethoxybenzene	117/103	II/III	+	+
benzonitrile	93/81	II/III	+	
methylpyrazine	31	III	+	
2-methylthiophene	15		+	
3-methylthiophene	17		+	
2-ethylthiophene	23		+	
(E) the series (E)	130		+	
(E)-theaspirate 0.5 dimethyl 4 methowy (0H)	69 70		+	
2,5 dimethy 4 - methoxy $(2n)$	10	111	I	
x-hexalactone	96	III	÷	
γ -nonalactone	142	III	+	
acetic acid	54^{-54}	III	+	+
3-methylbutanoic acid	94	III	+	
hexanoic acid	119	III	+	+
heptanoic acid	133	III	+	
octanoic acid	145	III	+	
nonanoic acid	154		+	
dodecanoic acid	175	111	+	

^a The peak numbers correspond to the numbers in Figures 1-3. ^b As identical retention data were found in HRGC and HRGC-MS analysis, only HRGC-MS has been inserted. Parentheses indicates contaminants of solvents. std = internal standards. (+) = identified by this technique using a reference sample.

M, 30 m, 0.0311-mm i.d.). On-column injection with a water-cooled injection system was employed. The conditions were as follows: temperature program, 5 min iso-

thermal at 60 °C, 60–240 °C, 2 °C/min; carrier gas, 1.0 mL/min He; temperature of ion source and all connection parts, 200 °C; electron energy, 70 eV; cathodic current, 0.8

Table II. Quantitative Distribution of Main Constituents of Cherimoya Fruit Volatiles

10- µg/kg o	-50 f pulp ^a	50-100 µg/kg of pulp ^a	100-500 μg/kg of pulp ^a	500-1000 μg/kg of pulp ^a	>1000 $\mu g/kg of pulp^a$
 α-thujene camphene α-terpinene γ-terpinene limonene 3-methylbutyl methylbutan 	3- loate	<i>p</i> -cymene	butyl butanoate 3-methylbutyl butanoate hexyl butanoate		
2-metyl-1-prop 2-methyl-3-bu 2-pentanol (E)-2-hexen-1- 2-ethyl-1-hexa benzyl alcohol	oanol ten-2-ol ol nol	2-methyl-2-butanol 1-pentanol 1-penten-3-ol (E)-3-penten-1-ol (Z)-2-penten-1-ol (Z)-3-hexen-1-ol α -terpineol		1-butanol linalool	3-methyl-1-butanol 1-hexanol
chrysanthenon	ne				

(Z)-linalool oxide, furanoid

^a Standard controlled capillary gas chromatographic determinations in fruit pulp, without consideration of calibration factors, i.e., F = 1.00 for all compounds.



Solvent extraction (pentane/dichloromethane, 2+1)

Concentration

Silica gel fractionation (pentane/diethylether gradient)

FRACTIONSI-III I I HRGC-MS HRGC HRGC-FT/IR

Figure 1. Scheme of separation, concentration and analysis of cherimoya (A. cherimolia, Mill.) volatiles.

mV; injection volumes, 0.1 μ L.

RESULTS AND DISCUSSION

In Figure 1 the different steps of our study on cherimoya volatiles are schematically outlined. The fruit pulp obtained after separation of the skin and the kernels was high-vacuum distilled; internal standards had been added before distillation. The aqueous distillate was then extracted with a pentane-dichloromethane (2:1) mixture. After careful concentration of the extract with the aid of a Vigreux column, the volatiles were preseparated by adsorption chromatography on silica gel employing a pentane-diethyl ether gradient (Schreier et al., 1979). Three fractions were eluted, which were analyzed by fused silica capillary gas chromatography (HRGC) as well as combined capillary gas chromatography-mass spectrometry (HRGC-MS) and on-line capillary gas chromatography-FTIR spectroscopy (HRGC-FTIR). The residue of the high-vacuum distillation was also investigated by HRGC and HRGC-MS

The results of HRGC separations of cherimoya volatiles in the three silica gel fractions are shown in Figures 2-4. In Table I the identities of the components determined by HRGC as well as on-line HRGC-MS and -FTIR are listed. In total, 208 volatiles could be identified by these techniques. Among them, 23 hydrocarbons, 58 esters, 54 alcohols, 47 carbonyls, and 26 volatiles of miscellaneous structures were found. Quantitatively, the major components among the volatiles consisted of alcohols such as



Figure 2. Fused silica capillary gas chromatographic separations of cherimoya volatiles (silica gel fractions I–III) after on-column injection using a J & W CW 20 M wide-bore column. Further conditions are given under Experimental Section. The peak numbers correspond to the numbers in Table I.



1-butanol, 3-methyl-1-butanol, 1-hexanol, and linalool and a series of butanoates and 3-methylbutyl esters. In Table II, the quantitative distribution of main constituents of cherimoya volatiles is demonstrated. The components listed in Table I and not represented in Table II were found in cherimoya pulp in amounts $<10 \ \mu g/kg$.

Most of the substances shown in Table II were detectable by the HRGC-FTIR technique (cf. Table I). Details of this study have already been published elsewhere (Herres et al., 1983). It must be pointed out that an amount in the range of approximately 5-20 ng/separated compound was needed to achieve satisfactory IR spectra. In Figure 5 the FTIR vapor-phase spectrum of butyl



Figure 5. Vapor-phase FTIR spectra of butyl (*E*)-2-butenoate (left) and butyl butanoate (right) obtained by HRGC-FTIR analysis of cherimoya volatiles.

(E)-2-butenoate is demonstrated as an example of positive identification in the lower concentration range; in contrast to that, the vapor-phase IR spectrum of a main component, butyl butanoate, is also shown in this figure.

As to the volatiles of the different chemical classes detected in cherimoya pulp, the following conclusions may be drawn. In the group of *hydrocarbons* a series of well-known terpenes have been identified. The concentrations of these volatiles were found to be in the range of $10-50 \ \mu g/kg$ of pulp or less.

The ester composition is characterized by a number of various butanoates and 3-methylbutyl esters. Among these compounds, the very uncommon (Z)- and (E)-2-pentenyl esters were identified. These esters exhibit "fruity" notes similar to those of hexenyl esters. The presence of numerous 3-methylbutyl esters and 3-methylbutanoates indicates a forced leucine metabolism as previously described for banana (Tressl and Drawert, 1973).

The butyl and 3-methylbutyl metabolism is also reflected in the composition of the *alcohol* group (cf. Tables I and II). Furthermore, 1-hexanol and the isomeric hexenols, all well-known as enzymic degradation products of unsaturated fatty acids (Galliard, 1975), were found in high amounts. Corresponding to the isomeric 2-pentenyl esters, in this fraction, (Z)- and (E)-2-penten-1-ol, both uncommon plant volatiles, should be mentioned.

Terpenoids were found in a great variety. Selected oxygenated monoterpenes are shown in Figure 6. In this group different volatiles, often found together with linalool, were detected, i.e., the well-known furanoid and pyranoid linalool oxides as well as tetrahydrofuran and tetrahydropyran derivatives such as 5-(methylethyl)-2methyl-2-vinyltetrahydrofuran, 2,2-dimethyl-5-(1methylpropenyl)tetrahydrofuran, and 2,6,6-trimethyl-2vinyltetrahydropyran (Figure 6a,b). The two last mentioned volatiles were first found in the distilled oil of lime (Kováts, 1963). Recently, the volatiles shown in Figure 6a,b were considered to be cleavage products of nonvolatile glycosidic precursors (Williams et al., 1982).

Furthermore, various bicyclic terpene ketones and alcohols were identified (Figure 6,c), which are known as constituents of different essential oils (Devon and Scott, 1972), i.e. camphor, pinocamphone, chrysanthenone, verbenone, myrtenal, and myrtenol.

The oxygenated terpenes shown in Figure 6d consist of well-known structures such as linalool, α -terpineol, 4-terpineol, carvone, and 1,8-cineole. Campholenaldehyde has been recently described in the essential oil of *Cistus ladanifer*, L. (Proksch et al., 1980).

In order to look for nondistillable aroma components, after solvent extraction and concentration, the residue of



Figure 6. Structures of various terpenoids identified in cherimoya fruit pulp. Identities (from left to right): a, 5-(methylethyl)-2-methyl-2-vinyltetrahydrofuran, 2,2-dimethyl-5-(1-methyl-propenyl)tetrahydrofuran, (Z)-linalool oxide, furanoid, 2,6,6-trimethyl-2-vinyltetrahydropyran, and (Z)-linalool oxide, pyranoid; b, (E)-linalool oxide, furanoid, and (E)-linalool oxide, pyranoid; c, camphor, pinocamphone, chrysanthenone, verbenone, myrtenal, and myrtenol; d, campholenaldehyde, linalool, α -terpineol, 4-terpinenol, carvone, and 1,8-cineole.

the high-vacuum distillate was also studied by HRGC-MS. 2,5-Dimethyl-4-methoxy-(2H)-furan-3-one was present among the distilled volatiles (peak no. 79, fraction III), but in contrast with mango (Pickenhagen et al., 1981; Idstein and Schreier, 1983), the corresponding hydroxylated compound was not detectable.

With this work we present for the first time a detailed analysis of the composition of volatiles in this aroma-impressive tropical fruit. As sensory evaluations were not carried out in this study it is difficult to answer the question which of the identified constituents may contribute to the cherimoya aroma. Obviously, the characteristic aroma is composed by a specific quantitative distribution of volatiles; among them the various esters should play an important role.

Registry No. 1-Phenoxybutene, 88296-28-0; toluene, 108-88-3; o-xylene, 95-47-6; m-xylene, 108-38-3; p-xylene, 106-42-3; ethylbenzene, 100-41-4; styrene, 100-42-5; 2,5-dimethylstyrene, 2039-89-6; 1,3-diethylbenzene, 141-93-5; propylbenzene, 103-65-1; camphene, 79-92-5; p-cymene, 99-87-6; limonene, 138-86-3; pmenth-1-ene, 5502-88-5; β -myrcene, 123-35-3; neoalloocimene, 7216-56-0; (E)-ocimene, 3779-61-1; (Z)-ocimene, 3338-55-4; αterpinene, 99-86-5; γ -terpinene, 99-85-4; terpinolene, 586-62-9; α -thujene, 2867-05-2; diethyl carbonate, 105-58-8; ethyl acetate, 141-78-6; butyl acetate, 123-86-4; 3-methylbutyl acetate, 123-92-2; 3-methyl-2-butenyl acetate, 1191-16-8; benzyl acetate, 140-11-4; linalyl acetate, 115-95-7; bornyl acetate, 76-49-3; terpinyl acetate, 80-26-2; butyl propanoate, 590-01-2; 3-methylbutyl propanoate, 105-68-0; linalyl propanoate, 144-39-8; propyl 2-hydroxypropanoate, 616-09-1; 3-methylbutyl 2-hydroxypropanoate, 19329-89-6; hexyl 2-methylpropanoate, 2349-07-7; benzyl 2methylpropanoate, 103-28-6; methyl butanoate, 623-42-7; ethyl butanoate, 105-54-4; 2-methylpropyl butanoate, 539-90-2; butyl butanoate, 109-21-7; 2-butenyl butanoate, 20279-26-9; 3methylbutyl butanoate, 106-27-4; pentyl butanoate, 540-18-1; 3-pentenyl butanoate, 88296-24-6; (Z)-2-pentenyl butanoate, 42125-13-3; (E)-2-pentenyl butanoate, 42125-30-4; hexyl butanoate, 2639-63-6; (Z)-3-hexenyl butanoate, 16491-36-4; (E)-2-hexenyl butanoate, 53398-83-7; benzyl butanoate, 103-37-7; butyl 2butenoate, 7299-91-4; 3-methylbutyl 2-butenoate, 25415-77-4; hexyl 2-butenoate, 19089-92-0; methyl 2-methylbutanoate, 868-57-5; hexyl 2-methylbutanoate, 10032-15-2; butyl 3-methylbutanoate, 109-19-3; 3-methylbutyl 3-methylbutanoate, 659-70-1; 3methyl-3-butenyl 3-methylbutanoate, 54410-94-5; pentyl 3methylbutanoate, 25415-62-7; (Z)-2-pentenyl 3-methylbutanoate, 88296-25-7; hexyl 3-methylbutanoate, 10032-13-0; (E)-3-hexenyl 3-methylbutanoate, 88296-26-8; (Z)-3-hexenyl 3-methylbutanoate, 35154-45-1; benzyl 3-methylbutanoate, 103-38-8; hexyl pentanoate, 1117-59-5; ethyl 2-hydroxy-4-methylpentanoate, 10348-47-7; ethyl 4-oxopentanoate, 539-88-8; methyl hexanoate, 106-70-7: 3methylbutyl hexanoate, 2198-61-0; (E)-2-pentenyl hexanoate,

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88296-27-9; hexyl hexanoate, 6378-65-0; methyl octanoate, 111-11-5; methyl decanoate, 110-42-9; ethyl decanoate, 110-38-3; methyl pentadecanoate, 7132-64-1; methyl octadecanoate, 112-61-8; methyl benzoate, 93-58-3; 3-methylbutyl benzoate, 94-46-2; 2-methyl-1-propanol, 78-83-1; 1-butanol, 71-36-3; 3-methyl-1butanol, 123-51-3; 2-butanol, 78-92-2; 2-methyl-2-butanol, 75-85-4; 2-methyl-3-buten-2-ol, 115-18-4; 1-pentanol, 71-41-0; (E)-2-penten-1-ol, 1576-96-1; (Z)-2-penten-1-ol, 1576-95-0; (E)-3-penten-1-ol, 764-37-4; 2-pentanol, 6032-29-7; 4-penten-2-ol, 625-31-0; 2methyl-2-pentanol, 590-36-3; 3-pentanol, 584-02-1; 1-penten-3-ol, 616-25-1; cyclopentanol, 96-41-3; 1-hexanol, 111-27-3; 2-ethyl-1hexanol, 104-76-7; (E)-3-hexen-1-ol, 928-97-2; (Z)-3-hexen-1-ol, 928-96-1; (E)-2-hexen-1-ol, 928-95-0; 1-hexen-3-ol, 4798-44-1; 1-heptanol, 111-70-6; 1-octanol, 111-87-5; (Z)-2-octen-1-ol, 26001-58-1; 1-nonanol, 143-08-8; 3-nonanol, 624-51-1; 1-decanol, 112-30-1; 1-dodecanol, 112-53-8; 1-tridecanol, 112-70-9; 1-tetradecanol, 112-72-1; 1-hexadecanol, 36653-82-4; 1-octadecanol, 112-92-5; 1-nonadecanol, 1454-84-8; benzyl alcohol, 100-51-6; 4-(methylethyl)benzyl alcohol, 536-60-7; 2-phenylethanol, 60-12-8; α-cadinol, 481-34-5; caryolan-1-ol, 52104-11-7; geraniol, 106-24-1; linalool, 78-70-6; (Z)-linalool oxide, furanoid, 5989-33-3; (E)-linalool oxide, furanoid, 34995-77-2; (Z)-linalool oxide, pyranoid, 14009-71-3; (E)-linalool oxide, pyranoid, 39028-58-5; mentha-2,8-dien-1-ol, 58940-40-2; mentha-?,?-dien-?-ol, 65391-05-1; methanol, 89-78-1; myrtenol, 515-00-4; nerol, 106-25-2; α-terpineol, 98-55-5; 4terpinenol, 562-74-3; 3-hydroxy-2-butanone, 513-86-0; 2-pentanone, 107-87-9; 3-penten-2-one, 625-33-2; 3-methylbutyl-2,4-pentandione, 10225-31-7; cyclohexanone, 108-94-1; 3,3,5-trimethylcyclohexanone, 873-94-9; 6-methyl-5-hepten-2-one, 110-93-0; 2-nonanone, 821-55-6; 2-tridecanone, 593-08-8; 3-tridecanone, 1534-26-5; 2-tetradecanone, 2345-27-9; 2-pentadecanone, 2345-28-0; 3-pentadecanone, 18787-66-1; 2-heptadecanone, 2922-51-2; 3-heptadecanone, 84534-29-2; 2-octadecanone, 7373-13-9; 3-nonadecanone, 27372-42-5; 2-eicosanone, 29703-52-4; 3-heneicosanone, 57755-77-8; 3methylacetophenone, 585-74-0; 4-methylacetophenone, 122-00-9; propiophenone, 93-55-0; butyrophenone, 495-40-9; benzophenone, 119-61-9; geranylacetone, 3796-70-1; camphor, 76-22-2; carvone, 99-49-0; chrysanthenone, 473-06-3; menthone, 89-80-5; pinocamphone, 547-60-4; verbenone, 80-57-9; 2-methyltetrahydrofuran-3-one, 3188-00-9; (E)-2-hexenol, 6728-26-3; (Z,E)-2,4-heptadienal, 59121-26-5; (E,E)-2,4-heptadienal, 4313-03-5; 2-ethyloctanol, 37596-38-6; dodecanal, 112-54-9; tetradecanol, 124-25-4; pentadecanal, 2765-11-9; benzaldehyde, 100-52-7; 2-methylbenzaldehyde, 529-20-4; 3-methylbenzaldehyde, 620-23-5; 4methylbenzaldehyde, 104-87-0; campholenealdehyde, 4501-58-0; myrtenal, 564-94-3; furfural, 98-01-1; 2,6,6-trimethyl--vinyltetrahydropyran, 7392-19-0; 2,2-dimethyl-5-(1-methylpropenyl)tetrahydrofuran, 7416-35-5; 5-(methylethyl)-2methyl-2-vinyltetrahydrofuran, 71635-17-1; 1,8-cineole, 470-82-6; phenol, 108-95-2; m-cresol, 108-39-4; thymol, 89-83-8; anethol, 104-46-1; 1,4-dimethoxybenzene, 150-78-7; benzonitrile, 100-47-0; methylpyrazine, 109-08-0; 2-methylthiophene, 554-14-3; 3methylthiophene, 616-44-4; 2-ethylthiophene, 872-55-9; benzothiazole, 95-16-9; (E)-theaspirane, 43126-22-3; 2,5-dimethyl-4methoxy-(2H)-furan-3-one, 4077-47-8; γ -hexalactone, 695-06-7; γ -nonalactone, 104-61-0; acetic acid, 64-19-7; 3-methylbutanoic acid, 503-74-2; hexanoic acid, 142-62-1; heptanoic acid, 111-14-8; octanoic acid, 124-07-2; nonanoic acid, 112-05-0; dodecanoic acid, 143-07-7.

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