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Characterization of the Key Aroma Compounds in Apricots (*Prunus armeniaca*) by Application of the Molecular Sensory Science Concept

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An aroma extract dilution analysis applied on an aroma distillate prepared from fresh apricots revealed (*R*)-γ-decalactone, (*E*)-β-damascenone, δ-decalactone, and (*R*/*S*)-linalool with the highest flavor dilution (FD) factors among the 26 odor-active compounds identified. On the basis of quantitative measurements performed by application of stable isotope dilution assays, followed by a calculation of odor activity values (OAVs), β-ionone, (*Z*)-1,5-octadien-3-one, γ-decalactone, (*E*,*Z*)-2,6-nonadienal, linalool, and acetaldehyde appeared with OAVs >100, whereas in particular certain lactones, often associated with an apricot aroma note, such as γ-undecalactone, γ-nonalactone, and δ-decalactone, showed very low OAVs (<5). An aroma recombinate prepared by mixing the 18 most important odorants in concentrations as they occurred in the fresh fruits showed an overall aroma very similar to that of apricots. Omission experiments indicated that previously unknown constituents of apricots, such as (*E*,*Z*)-2,6-nonadienal or (*Z*)-1,5-octadien-3-one, are key contributors to the apricot aroma.

KEYWORDS: Aroma; apricot; molecular sensory concept; (*E*,*Z*)-2,6-nonadienal; (*Z*)-1,5-octadien-3-one

INTRODUCTION

Like many stone fruits, apricots are appreciated by consumers all over the world and, consequently, have gained great economic importance. The fruits are presently cultivated in all Mediterranean countries and in South Africa as well as in South and North America, mainly in California. The crop is either marketed fresh, but also used as canned and dried fruit, or is manufactured into juice.

Apart from color, sweetness, and texture, apricots are especially popular for their characteristic aroma. However, although flavor is one of the most important criteria in the evaluation of fruit quality, investigations on the volatile fraction and, in particular, the odor-active compounds of apricot are rather scarce. The first comprehensive studies on apricot volatiles were performed by Tang and Jennings about 40 years ago (*1*, *2*) and led to the identification of γ-octalactone, γ-decalactone, γ-dodecalactone, δ-decalactone, linalool, α-terpineol, geraniol, myrcene, and limonene as the predominant volatile constituents. Further studies undertaken by Rodriguez et al. (*3*), Guichard and Souty (*4*), and Toth-Markus et al. (*5*) as well as Bolzoni et al. (*6*), Takeoka et al. (*7*), and Gómez and Ledbetter (*8*) have considerably increased the number of volatiles identified in apricot, and >200 compounds have been listed so far (*9*).

The human odorant receptors present in the nasal cavity show considerable selectivity and high differences in sensitivity toward organic volatiles, and, thus, the evaluation of odor thresholds is a good tool to select potent aroma compounds from the bulk of odorless or less odor-active volatiles. GC−olfactometry uses the concept of "ranking by odor thresholds" and, thus, studies using GC−olfactometry on serial dilutions of aroma distillates (*10*), such as CHARM analysis or aroma extract dilution analysis (AEDA), have clearly shown that only if the concentration of a given volatile exceeds its odor threshold will this compound interact with the human odorant receptors and, consequently, participate in the creation of the respective aroma impression in the brain. Before 1980, however, no attempts were made to investigate the volatiles of apricot with regard to their aroma activity and, surprisingly, no application of dilution to odor threshold techniques, such as the AEDA, on apricots is available in the current literature.

In a few studies quantitative data were related to the odor thresholds of individual compounds (*5*, *7*). On the basis of the calculation of odor activity values (OAVs; ratio of concentration to odor thresholds in water), these authors suggested that, in particular, β-ionone, linalool, γ-decalactone, hexanal, (*E*)-2-hexenal, and geraniol should be considered as key odorants of apricot. However, these results are somewhat preliminary because quantitative data were obtained by GC-FID measurements either without the use of internal standards or using only one internal standard for the entire set of volatiles. Moreover, no aroma reconstitution experiments based on the results of quantitative data have been performed, which are, however,

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necessary to confirm the correctness of the quantitative data (*10*). Such aroma recombination studies based on the real concentrations of the respective odorants in the food itself are among the most reliable tools to evaluate whether a mixture of odorants with a variety of odor qualities will finally be able to mimic the odorant receptor responses. This approach, which can be assigned as "molecular sensory science" or "sensomics", has already successfully been used to confirm the key odorants of many foods and, most recently, to identify the aroma and taste compounds of a black tea beverage (*11*, *12*). It is a valuable tool, in particular, to address the challenge that single key odorants of a certain food do not smell like the food itself, but a distinct mixture may perfectly match the overall food aroma.

Consequently, the aim of this study was, first, to locate and characterize the most odor-active compounds in an extract isolated from fresh apricots by application of the AEDA. In a second step, the key odorants were quantified by means of stable isotope dilution analyses (SDIAs) and their OAVs were calculated. Finally, aroma recombinates based on the concentrations of each aroma compounds as occurring in apricot were prepared and evaluated by aroma profile analysis. On the basis of this approach the sensory active volatiles are selected from the total volatile metabolites (the metabolome) of the fruit, and a pattern of key aroma compounds becomes available, representing the blueprint of compounds evoking the human odorant receptor responses and, finally, creating the overall aroma impression in the brain.

MATERIALS AND METHODS

Apricots. Fully ripe French apricots (cv. Bergeron) were purchased from a local store (Olympia Fruchthaus, Munich, Germany). For the aroma profile analysis and the AEDA as well as for the quantification of (*Z*)-3-hexenal and acetaldehyde, a new batch of fresh fruits of the same variety was always used.

For the quantitation of the remaining odorants, fruits were frozen with liquid nitrogen, shrink-wrapped in plastic film, and stored at −20 °C. All fruits, either fresh or deep-frozen, were taken from the same variety of apricots, but from different batches. To avoid enzymatic reactions, care was taken to not use thawed fruits for volatile isolation before aqueous $CaCl_2$ was added (see below).

Chemicals. 4-Bromo-1-butene, 3-chloroperoxybenzoic acid, deuterium oxide, 1,4-dichloro-2-butyne, ethyl magnesium bromide (1 mol/L in tetrahydrofuran), 3-hexyn-1-ol, and sodium hydride were obtained from Aldrich (Taufkirchen, Germany). Methyl octanoate was obtained from Fluka. Dess-Martin-periodinane and Wilkinson's catalyst were obtained from Lancaster Synthesis (Ward Hill, MA). Deuterium and liquid nitrogen were obtained from Linde (Munich, Germany). Calcium chloride, citric acid, 1,3-cyclohexanedione, dichloromethane, diethyl ether, ethanol, fructose, glucose, hydrochloric acid (37%), lithium aluminum hydride, pentane, potassium bromide, potassium iodide, potassium hydroxide, sucrose, sea sand, silica gel, sodium boronhydride, sodium carbonate, sodium hydrogen carbonate, anhydrous sodium sulfate, sodium thiosulfate−pentahydrate, sorbitol, sulfuric acid, tetrahydrofuran, and toluene were obtained from VWR (Darmstadt, Germany). Malic acid and pectin were obtained from Roth (Karlsruhe, Germany).

Diethyl ether, dichloromethane, and pentane were freshly distilled prior to use.

Reference Aroma Compounds. The following reference compounds were obtained from the suppliers given in parentheses: γ-decalactone, δ-decalactone, γ-dodecalactone, hexanal, (*E*)-2-hexenal, (*R*)-linalool, 3-methylbutanoic acid, (*E*,*Z*)-2,6-nonadienal, γ-nonalactone, (*E*)-2-nonenal, γ-octalactone, (*E*)-2-octenal, (*E*,*E*)-2,4-decadienal (Aldrich, Sigma-Aldrich Chemie, Taufkirchen, Germany); butanoic acid, hexanoic acid, hexyl acetate, (*R*,*S*)-linalool, 2-methylbutanoic acid, pentanoic acid (Fluka, Neu-Ulm, Germany); (*Z*)-3-hexenyl acetate, 1-octen-3-one (Lancaster, Mühlheim am Main, Germany); acetic acid, eugenol, 4-methoxyphenol (Merck, Darmstadt, Germany); geraniol (Roth, Karlsruhe, Germany). (*E*)-β-Damascenone and β-ionone were gifts from Symrise (Holzminden, Germany).

Synthesis of *trans*-4,5-Epoxy-(*E*)-2-decenal. 3-Chloroperoxybenzoic acid (1.8 g, 10 mmol) acid was dissolved in dichloromethane (80 mL) and added in nine equal portions to a solution of (*E*,*E*)-2,4-decadienal (936 mg, 6.2 mmol in 10 mL of dichloromethane). The mixture was stirred at room temperature for 140 min and finally left overnight (15 h) at −20 °C. The solution was dried over sodium sulfate and concentrated to 2 mL at 45 °C using a Vigreux column. The target compound was purified by column chromatography (water-cooled column, 20 cm × 1 cm) using modified silica gel 60 (*13*).

MS-EI (*m*/*z* in %): 68 (100), 81 (35), 41 (23), 39 (17), 55 (15), 43 (14), 69 (12), 57 (8). MS-CI (*m*/*z* in %): 153 (100), 154 (10), 169 (7).

The following reference compounds were synthesized according to the literature cited: (*Z*)-3-hexenal (*14*), 3-methyl-2,4-nonandione (*15*), and (*Z*)-1,5-octadien-3-one (*14*).

Isotopically Labeled Internal Standards. *[$^2H_3$]-β-Ionone.* β-Ionone (39 mg, 0.2 mmol), dissolved in dry tetrahydrofuran (1 mL), was added to sodium hydride (10 mg, 0.4 mmol) maintained in an atmosphere of nitrogen. Deuterium oxide (1 mL, 0.056 mol) was added, and the mixture was stirred for 24 h in a closed flask at room temperature. The mixture was extracted with diethyl ether (2 × 20 mL), dried over sodium sulfate, and subjected to high vacuum distillation (*16*) to remove nonvolatile compounds.

MS-EI (*m*/*z* in %): 180 (100), 46 (21), 181 (12), 91(8), 138 (7), 93 (7), 162 (6).

MS-CI (*m*/*z* in %): 196 (100), 197 (14).

[$^2H_2$]-δ-Decalactone. 4-Bromo-1-butene (3.37 g, 25 mmol), 1,3-cyclohexandione (2.88 g, 25 mmol), and potassium hydroxide (1 g, 25 mmol) were dissolved in dioxane/water (1:1, v/v, 25 mL) and refluxed for 7 h (*17*). Aqueous potassium hydroxide (25 mL; 30 g/L) was added, and the mixture was extracted with diethyl ether (3 × 50 mL). The organic layer was discarded, and the aqueous layer was adjusted to pH 4.0 with hydrochloric acid and extracted with diethyl ether (3 × 50 mL). The combined organic layers were dried over sodium sulfate and, after filtration, the solvent was distilled off. The residue (3.65 g) was refluxed for 30 h in an aqueous Na_2CO_3 (300 g/L; 37.5 mL). The mixture was adjusted to pH 3.0 with hydrochloric acid (5 mol/L) and extracted with diethyl ether (3 × 50 mL). The combined organic layers were dried over sodium sulfate, and the solvent was distilled off, yielding 5-oxo-dec-9-enoic acid (0.2 g, 1.1 mmol). Sodium borohydride (0.85 g, 25 mmol) was added in small portions, followed by aqueous potassium hydroxide (50 mL; 30 g/L). The mixture was stirred at 40 °C for 9 h, adjusted to pH 1.0 with HCl (30%), and refluxed for 30 min. The aqueous solution was cooled to room temperature and extracted with diethyl ether (3 × 50 mL). The combined organic layers were dried over sodium sulfate, and the solvent was distilled off, yielding δ-dec-9-enolactone. The crude product was purified by column chromatography (water-cooled column, 20 cm × 1 cm i.d.) using silica gel 60 adjusted to 7% water content. After the column had been flushed with pentane (150 mL), the target compound was eluted with pentane/diethyl ether (60:40, v/v). The δ-dec-9-enolactone was dissolved in toluene (20 mL), mixed with Wilkinson's catalyst [tris(triphenylphosphine)rhodium(I) chloride] (300 mg, 0.32 mmol) and deuterated in an autoclave at 5 bar for 90 min. The target compound was purified by column chromatography (water-cooled column, 20 cm × 1 cm) on silica gel 60. Elution was performed with pentane/diethyl ether (60:40, v/v).

MS-EI (*m*/*z* in %): 99 (100), 71 (33), 42 (25), 70 (22), 55 (16), 43 (12), 41 (12), 114 (10).

MS-CI [*m*/*z* in %): 173 (100), 174 (12), 155 (2).

[$^2H_4$]-trans-4,5-Epoxy-(E)-2-decenal. 3-Hexyn-1-ol (2.0 g, 20.4 mmol), dissolved in toluene (15 mL), was deuterated in the presence of Wilkinson's catalyst (750 mg, 0.81 mmol) under a slight pressure of deuterium for 24 h, yielding [$^2H_4$]hexanol. The crude product was purified by column chromatography (water-cooled column; 20 cm × 1 cm i.d.) on silica gel in pentane. Elution was performed with diethyl ether (300 mL). To remove nonvolatile compounds, the orange solution was subjected to high-vacuum distillation (*16*) and the solvent was finally distilled off. The [$^2H_4$]hexanol (2.1 g, 19.8 mmol) was dissolved in dichloromethane (20 mL) and added dropwise to a solution of Dess-

Martin-periodinane (9 g, 21.2 mmol, in 20 mL of dichloromethane). After 16 h of stirring, diethyl ether (100 mL) was added and the solution was treated with sodium thiosulfate (100 mL, 1 mol/L, saturated with sodium hydrogen carbonate) until the organic layer was clear. The organic layer was washed again with a solution of sodium thiosulfate (50 mL, 1 mol/L, saturated with sodium hydrogen carbonate), followed by a saturated solution of sodium hydrogen carbonate (100 mL) and, finally, with water (100 mL). The organic layer was dried over sodium sulfate, and the solvent was distilled off, yielding [$^2H_4$]hexanal.

For the synthesis of 1-methoxy-but-1-en-3-yne, a solution of potassium hydroxide (10 g, 0.18 mol) in methanol (33 mL, 0.8 mol) was heated to 65 °C. With continuous stirring, 1,4-dichloro-2-butyne (10.3 g, 83.7 mmol) was dropwise added to the solution, and the mixture was stirred for another 60 min at room temperature. Water (20 mL) was added, and the solution was extracted with diethyl ether (3 × 50 mL). The organic layer was dried over calcium chloride and subjected to high-vacuum distillation for purification. The solvent was finally distilled off, and the residue was taken up in tetrahydrofuran. The 1-methoxy-but-1-en-3-yne (1 g, 12 mmol) obtained was dissolved in THF (5 mL) and dropwise added to ethyl magnesium bromide (12 mmol dissolved in 12 mL of THF) held at 40 °C. The mixture was stirred for 60 min. Then, [$^2H_4$]hexanal (0.86 g, 8 mmol, dissolved in 5 mL of THF) was dropwise added, and the solution was stirred for another 2 h. After the addition of ethanol (0.8 mL, 13.5 mmol) and further stirring for 20 min, lithium aluminum hydride (0.4 g, 10 mmol) was added in small portions. The mixture was stirred for 15 h, and ethyl acetate (1.2 mL), followed by water (5.6 mL) and sulfuric acid (28 mL, 4 mol/L), was added. The organic layer was separated, and the aqueous phase was extracted with pentane/dichloromethane (30 mL, 1:1, v/v). The combined organic layers were washed with aqueous sodium carbonate (10% w/w, 250 mL), then with water (50 mL) and finally dried over sodium sulfate. The solvent was distilled off to yield [$^2H_4$]-(*E*,*E*)-2,4-decadienal (1.1 g). The [$^2H_4$]-(*E*,*E*)-2,4-decadienal was finally oxidized into [$^2H_4$]-*trans*-4,5-epoxy-(*E*)-2-decenal with 3-chloroperoxybenzoic acid (1.8 g, 10 mmol) as described above for the unlabeled compound.

MS-EI (*m*/*z* in %): 68 (100), 81 (31), 39 (11), 69 (10), 43 (8), 45 (8), 44 (7).

MS-CI (*m*/*z* in %): 157 (100), 158 (10).

The following isotopically labeled internal standards were synthesized according to the literature cited: [$^2H_2$]-butanoic acid (*17*), [$^2H_6$]-(*E*)-β-damascenone (*18*), [$^2H_2$]-γ-decalactone (*19*), [$^2H_2$]-γ-dodecalactone (*19*), [$^2H_2$]-geraniol (A. Fischer, personal communication), [$^2H_4$]-hexanal (*20*), [$^2H_2$]-(*E*)-2-hexenal (*21*), [$^2H_2$]-(*Z*)-3-hexenal (*22*), [$^{13}C_2$]-(*Z*)-3-hexenyl acetate (*23*), [$^2H_{2-4}$]-hexyl acetate (*23*), [$^2H_2$]-linalool (*24*), [$^2H_3$]-2-methoxyphenol (*25*), [$^2H_2$]-3-methylbutanoic acid (*26*), [$^2H_3$]-3-methyl-2,4-nonandione (*22*), [$^2H_2$]-(*E*,*Z*)-2,6-nonadienal (*22*), [$^2H_2$]-γ-nonalactone (*19*), [$^2H_2$]-(*E*)-2-nonenal (*22*), [$^2H_2$]-1-octen-3-one (*22*), [$^2H_2$]-(*Z*)-1,5-octadien-3-one (*22*), [$^2H_2$]-γ-octalactone (*27*), [$^2H_{2-4}$]-4-propyl-2-methoxyphenol (*28*).

[$^{13}C_2$]-Acetaldehyde and [$^2H_3$]-acetic acid were purchased from Aldrich (Steinheim, Germany).

Concentrations of Labeled Compounds. Because most of the syntheses were performed at a microscale level, common purification procedures, such as distillation or crystallization, were not possible. To determine the yields and exact concentrations, the following approach was used: First, an FID response factor was determined by GC analysis of a solution containing defined amounts of the respective unlabeled compound and methyl octanoate as a reference standard. In a second step, a defined amount of methyl octanoate was added to a defined volume of the solution containing the labeled compound. The resulting mixture was analyzed by GC-FID, and the concentration of the labeled compound was calculated from the peak areas of the GC chromatogram, using the FID response factor determined for the unlabeled compound.

Isolation of Volatiles. Fresh apricots (250 g) were sliced and blended with saturated calcium chloride solution (250 mL) to inhibit enzymic reactions (*29*). After the suspension had been adjusted to pH 3.3 (natural pH of apricots), volatiles were isolated using the solvent-assisted flavor evaporation technique (SAFE) (*16*). The aqueous distillate was extracted with diethyl ether (4 × 50 mL), and, to separate the acidic volatiles from the neutral-basic fraction, the solvent extract was treated with aqueous sodium bicarbonate (0.5 mol/L, 4 × 50 mL). The combined aqueous solutions were adjusted to pH 2 with hydrochloric acid (2 mol/L) and extracted with diethyl ether (4 × 50 mL) to obtain the acidic compounds (AF).

The solutions containing either the acidic (AF) or the neutral-basic (NBF) fraction were concentrated to 2 mL at 40 °C using a Vigreux column. The extracts were transferred into a microflask and further concentrated to 200 μL using a microdistillation column.

High-Resolution Gas Chromatography (HRGC) and HRGC−Olfactometry (HRGC-O). HRGC was performed by means of a gas chromatograph type 8000 series (Fisons Instruments, Mainz, Germany) using the following capillary columns: DB-5 (30 m × 0.25 mm i.d.; 0.25 μm film thickness; J&W Scientific, Folsom, CA); DB-FFAP (30 m × 0.32 mm i.d.; 0.25 μm film thickness; J&W Scientific); OV-1701 (30 m × 0.25 mm i.d.; 0.25 μm film thickness; J&W Scientific); BGB-176 (30 m × 0.25 mm i.d.; 0.25 μm film thickness; J&W Scientific). The temperature programs used were as follows:

$$\text{DB-5: } 40\ ^\circ\text{C/1 min} \xrightarrow{7\ ^\circ\text{C/1 min}} 110\ ^\circ\text{C} \xrightarrow{5\ ^\circ\text{C/min}} 180\ ^\circ\text{C} \xrightarrow{10\ ^\circ\text{C/min}} 240\ ^\circ\text{C/10 min}$$

$$\text{DB-5: } 40\ ^\circ\text{C/1 min} \xrightarrow{7\ ^\circ\text{C/1 min}} 180\ ^\circ\text{C} \xrightarrow{10\ ^\circ\text{C/min}} 240\ ^\circ\text{C/10 min}$$

$$\text{OAV-1701: } 40\ ^\circ\text{C/1 min} \xrightarrow{8\ ^\circ\text{C/min}} 240\ ^\circ\text{C/10 min}$$

$$\text{BGB-176: } 40\ ^\circ\text{C/1 min} \xrightarrow{10\ ^\circ\text{C/min}} 100\ ^\circ\text{C} \xrightarrow{6\ ^\circ\text{C/min}} 225\ ^\circ\text{C/10 min}$$

For HRGC-O, the effluent was split evenly at the end of the column between a flame ionization detector (FID) and a heated (180 °C) sniffing port using a Y-shaped glass splitter and uncoated deactivated fused silica capillaries (50 cm, 0.1 mm i.d. as transfer lines). Helium, adjusted to a flow rate of 1.5 mL/min, served as the carrier gas. Retention indices (RI) were calculated from the retention times of *n*-alkanes by linear interpolation.

AEDA. Flavor dilution (FD) factors were determined by AEDA (*7*) of fractions NBF and AF, respectively, using capillary columns DB-5, FFAP, or OV-1701. Extracts were diluted stepwise with solvent in a 1:1 ratio, and each dilution was analyzed by HRGC-O (injection volume = 1 μL). The AEDA was performed by three experienced assessors. These underwent a GC-O training including sniffing of about 50 reference compounds in amounts adjusted to 5-fold above their odor thresholds in air.

HRGC−Mass Spectrometry (HRGC-MS). For compound identification, mass spectra were generated by means of an MAT 95 S mass spectrometer (Finnigan, Bremen, Germany) at 70 eV in the electron ionization (EI) mode and at 115 eV in the chemical ionization (CI) mode (reagent gas = isobutane) using the FFAP and DB-5 capillaries.

SIDA. Extracts of the fruits (fresh or frozen) were prepared as described under Isolation of Volatiles. Various amounts of fruit purée (20−600 g) were used, depending on the amounts of the target compounds estimated in preliminary experiments. After the fruit samples had been spiked with defined amounts of the labeled standards (resulting in a concentration of 1−5 μg/mL of each compound in the aroma extract), the samples were stirred for 60 min for equilibration. To isolate the volatile fraction, a SAFE distillation (*16*) and solvent extraction were performed as described above.

For the quantitation of acetaldehyde by headspace gas chromatography−mass spectrometry, the fruit samples (50 g) and the labeled acetaldehyde were added to a 200 mL Erlenmeyer flask, which was tightly sealed with a septum, and the mixture was stirred for 45 min at room temperature until equilibrium was reached.

Quantitation of aroma compounds was performed by means of three different HRGC-MS systems using the FFAP, DB-5, and OV-1701 capillaries: Acids and lactones (except γ-nonalactone and γ-undecalactone) were quantified using a gas chromatograph Varian GC 3800 (Varian, Darmstadt, Germany) coupled to an ion trap mass spectrometer Saturn 2000 (Varian). Quantitation of the remaining compounds was performed by means of a two-dimensional HRGC-MS system consisting of a gas chromatograph Trace 2000 series (Thermo Quest, Egelsbach, Germany) coupled to a gas chromatograph Varian GC 3800. Mass

Table 1. Isotopically Labeled Standards, Ions Selected, and Response Factors Used in the Isotope Dilution Assays of the 30 Key Apricot Aroma Compounds

odorant	ion (*m*/*z*)	labeled standard	ion (*m*/*z*)	RF[a]
acetaldehyde	45	[$^{13}C_2$]-acetaldehyde	47	0.88
butanoic acid	89	[$^{2}H_2$]-butanoic acid	91	0.83
(*E*)-β-damascenone	191	[$^{2}H_{5-7}$]-(*E*)-β-damascenone	196–198	0.73
γ-decalactone	171	[$^{2}H_2$]-γ-decalactone	173	0.60
δ-decalactone	171	[$^{2}H_2$]-δ-decalactone	173	1.03
γ-dodecalactone	199	[$^{2}H_2$]-γ-dodecalactone	201	0.62
trans-4,5-epoxy-(*E*)-2-decenal	139	[$^{2}H_4$]-*trans*-4,5-epoxy-(*E*)-2-decenal	143	0.98
acetic acid	61	[$^{2}H_3$]-acetic acid	64	0.78
eugenol	165	[$^{2}H_{4-6}$]-4-propyl-2-methoxyphenol	169–171	1.02
geraniol	137	[$^{2}H_2$]-geraniol	139	0.92
hexanal	101	[$^{2}H_4$]-hexanal	105	0.76
hexanoic acid	117	[$^{2}H_2$]-3-methylbutanoic acid	105	0.99
(*E*)-2-hexenal	99	[$^{2}H_2$]-(*E*)-2-hexenal	101	0.80
(*Z*)-3-hexenal	81	[$^{2}H_2$]-(*Z*)-3-hexenal	83	0.62
(*Z*)-3-hexenylacetate	143	[$^{13}C_2$]-(*Z*)-3-hexenylacetate	145	0.88
hexylacetate	145	[$^{2}H_{2-5}$]-hexylacetate	147–150	0.91
β-ionone	193	[$^{2}H_3$]-β-ionone	196	0.87
linalool	137	[$^{2}H_2$]-linalool	139	0.92
2-methoxyphenol	125	[$^{2}H_3$]-2-methoxyphenol	128	1.04
2- and 3-methylbutanoic acid	103	[$^{2}H_2$]-3-methylbutanoic acid	105	0.86
3-methyl-2,4-nonandione	171	[$^{2}H_3$]-3-methyl-2,4-nonandione	174	0.83
(*E*,*Z*)-2,6-nonadienal	139	[$^{2}H_2$]-(*E*,*Z*)-2,6-nonadienal	141	0.97
γ-nonalactone	157	[$^{2}H_2$]-γ-nonalactone	159	0.74
(*E*)-2-nonenal	141	[$^{2}H_2$]-(*E*)-2-nonenal	143	0.90
(*E*)-2-octenal	127	[$^{2}H_2$]-(*E*)-2-nonenal	143	0.91
1-octen-3-one	127	[$^{2}H_2$]-1-octen-3-one	129	0.61
(*Z*)-1,5-octadien-3-one	125	[$^{2}H_2$]-(*Z*)-1,5-octadien-3-one	127	0.96
γ-octalactone	143	[$^{2}H_2$]-γ-octalactone	145	0.49
pentanoic acid	103	[$^{2}H_2$]-3-methylbutanoic acid	105	0.82
γ-undecalactone	185	[$^{2}H_2$]-γ-undecalactone	187	0.48

[a] MS response factor determined by analyzing defined mixtures of the analyte and the internal standard.

spectra were recorded using a Varian Saturn 2000 mass spectrometer. Acetaldehyde was quantified HRGC-MS using headspace samples and a gas chromatograph CP-9001 (Chrompack, Frankfurt, Germany) coupled to a quadrupole mass spectrometer INCOS XL (Finnigan MAT, Bremen, Germany). All mass spectra were recorded in the CI mode with methanol as the reagent gas and using the temperature programs mentioned above.

For each compound, a calibration factor was determined by analyzing mixtures of defined amounts of the labeled and unlabeled compound in five different mass ratios (1:5, 1:3, 1:1, 3:1, 5:1) by HRGC-MS. The MS response factors, which were calculated from the peak areas and the amounts of labeled and unlabeled compound, are summarized in **Table 1**.

Determination of Enantiomeric Distributions. The enantiomeric ratios in linalool, γ-octalactone, γ-decalactone, and γ-dodecalactone were determined by two-dimensional gas chromatography−mass spectrometry using the chiral BGB-176 capillary as the second column according to the described procedure (*24*).

Aroma Profile Analysis. Aroma profile analyses were performed by a trained sensory panel consisting of 16 panelists as previously described (*11*). The following aroma descriptors, represented by the compounds given in parentheses, were chosen for sensory evaluation, and their intensities were ranked on a seven-point scale (steps of 0.5) from 0 (not perceivable) to 3 (strongly perceivable): fruity/fresh (acetaldehyde); peach-like (γ-decalactone, γ-dodecalactone); fruity/apple-like [(*E*)-β-damascenone]; banana-like (hexyl acetate); coconut-like (γ-octalactone, δ-decalactone); green/grassy [hexanal, (*Z*)-3-hexenal]; mushroom-like (1-octen-3-one); cucumber-like [(*E*,*Z*)-2,6-nonadienal]; flowery/citrus-like (linalool); geranium-like [(*Z*)-1,5-octadien-3-one], metallic [*trans*-4,5-epoxy-(*E*)-2-decenal]; violet-like (β-ionone); and rose-like (geraniol). The judgments of the panelists were averaged.

Aroma Reconstitution Experiments. As the reference, fresh apricots were blended and the samples (20 mL each) were placed in glass vessels (total volume = 45 mL). The sensory evaluation was finished about 20 min after blending of the fruits. Aroma models containing the following compounds in concentration levels equal to those determined in apricots were prepared: acetaldehyde, (*E*)-β-damascenone, γ-decalactone, δ-decalactone, γ-dodecalactone, *trans*-4,5-epoxy-(*E*)-2-decenal, geraniol, hexanal, (*Z*)-3-hexenal, hexyl acetate, β-ionone, linalool, 3-methyl-2,4-nonandione, (*E*,*Z*)-2,6-nonadienal, (*E*)-2-nonenal, (*Z*)-1,5-octadien-3-one, γ-octalactone, 1-octen-3-one. As the matrix an aqueous solution of 1.7% glucose, 0.9% fructose, 5.1% sucrose, 0.8% sorbitol, 1% malic acid, 0.4% citric acid, and 1% pectin in tap water was prepared to simulate the natural content of carbohydrates and acids in apricots (*30*).

The model mixture and the freshly mashed apricots were presented to the sensory panel and were orthonasally evaluated. In one session, the aroma profile of the apricots was evaluated, in another session the aroma profile of the recombinate was judged. In a third session, the similarity of the recombinate and the fruit puree was compared. All evaluations were performed in triplicates.

Omission Experiments. A second model mixture omitting (*Z*)-1,5-octadien-3-one, (*E*,*Z*)-2,6-nonadienal, 1-octen-3-one, *trans*-4,5-epoxy-(*E*)-2-decenal, and (*E*)-2-nonenal was prepared (model II). Together with the original recombinate (model I), it was presented to the sensory panel in a triangle test in which each panelist had to evaluate two triangle rows. The panelists were asked to identify the odd sample, and the significance of the difference was calculated (*31*).

RESULTS AND DISCUSSION

Odor-Active Compounds in Apricots. The entire volatiles from fresh apricots, isolated by extraction with diethyl ether and SAFE distillation, were evaluated by the sensory panel by smelling a drop of the etherial extract on a strip of filter paper as done by perfumers. After evaporation of the solvent, all 10 panelists agreed that the distillate evoked the characteristic odor of apricot, thereby indicating that the method used for aroma isolation was appropiate.

Application of HRGC−olfactometry on an aliquot of the aroma extract equal to ~1.25 g of fresh fruits (250 g of fruits

Table 2. Important Aroma Compounds (FD ≥ 8) Identified in an Aroma Distillate Prepared from Fresh Apricots

no.	aroma compound[b]	odor quality[c]	RI[a] on FFAP	RI[a] on DB-5	RI[a] on OV-1701	FD[d]	earlier identified as volatile in apricots
1	(*Z*)-3-hexenal	green/grassy	1144	800	885	64	
2	hexyl acetate	banana-like	1271	1010	1086	8	*4*
3	1-octen-3-one	mushroom-like	1295	975	1070	32	
4	(*Z*)-3-hexenyl acetate	banana-like	1312	1010	1081	8	*4*
5	(*Z*)-1,5-octadien-3-one	geranium-like	1370	980	1099	128	
6	unknown	fruity/citrus-like	1393	nd[f]	nd	16	
7	(*E*)-2-octenal	fatty, green	1420	1093	1165	8	*33*
8	acetic acid	vinegar-like	1443	600	775	16	*1*
9	(*E*)-2-nonenal	fatty	1533	1160	1280	8	*7*
10	(*R*/*S*)-linalool	flowery/citrus-like	1540	1105	1200	256	*1*
11	butanoic acid	sweaty	1619	821	990	32	*5*
12	2- and 3-methylbutanoic acid[e]	sweaty	1662	878	1030	32	*1*
13	unknown	leather-like	1685	1190	nd	16	
14	3-methyl-2,4-nonandione	green, hay-like	1711	1247	1380	8	
15	unknown	metallic	1732	nd	nd	16	
16	(*E*)-β-damascenone	fruity/apple-like	1802	1380	1498	512	*34*
17	geraniol	rose-like	1835	1256	1590	16	*3*
18	2-methoxyphenol	smoky, sweet	1860	1095	1225	32	
19	unknown	coconut-like	1875	1321	nd	16	
20	(*R*/*S*)-γ-octalactone	coconut-like	1910	1268	1480	128	*1*
21	β-ionone	violet-like	1930	1480	1630	16	*34*
22	*trans*-4,5-epoxy-(*E*)-2-decenal[e]	metallic	2000	1390	1570	8	
23	(*R*)-γ-decalactone	peach-like	2140	1471	1700	2048	*1*
24	eugenol	clove-like	2156	1360	1505	8	
25	δ-decalactone[e]	coconut-like	2196	1490	1740	256	*2*
26	(*R*)-γ-dodecalactone	peach-like	2380	1680	1910	8	*2*

[a] Retention index. [b] Identification was performed on the basis of a comparison with reference compounds using the following criteria: retention index on three different capillary columns, odor quality and odor threshold perceived at the sniffing port, mass spectra in the EI- and CI-mode on two different capillary columns. [c] Odor quality perceived at the sniffing port. [d] Flavor dilution factor. [e] The stereochemistry was not determined. [f] Not determined.

→ 200 μL of distillate → 1 μL for HRGC-O) led to the detection of 26 odor-active regions in the FD factor range of 8−2048 (**Table 2**). A great variety of odor qualities, such as green/grassy, flowery, fruity/peach-like, coconut-like, mushroom-like, or cucumber-like were detected, but no aroma quality of a single odorant resembled the overall apricot aroma. Sniffing of serial dilutions of the aroma extract revealed the highest FD factor (2048) for a fruity/peach-like smelling compound (no. **23**). Somewhat lower FD factors were determined for compounds with fruity/apple-like (no. **16**), flowery/citrus-like (no. **10**), coconut-like, geranium-like, and green/grassy odor qualities (**Table 2**).

For preliminary identifications, the odor quality perceived at the sniffing port and the retention index on three stationary columns are important parameters. Comparison of these data with an in-house database containing >600 food aroma compounds suggested a structure for the respective target compound. To unequivocally identify the compounds responsible for the odors detected in the respective area, the neutral-basic volatiles isolated from 1 kg of fresh apricots were separated by column chromatography on silica according to polarity (*13*). The odorants were then located by GC−olfactometry in the six fractions obtained, and mass spectra in the MS-EI and the MS-CI mode were recorded at the respective retention index. In addition to the mass spectra, and to avoid wrong identifications caused, for example, by coeluting compounds, also the odor potency of a target molecule (ratio of peak area to FD factor) was used as further criterion in the comparison with the reference compounds. The compounds with the highest FD factors could, thus, be identified as γ-decalactone (no. **23**), (*E*)-β-damascenone (no. **16**), linalool (no. **10**), and δ-decalactone (no. **25**) followed by γ-octalactone (no. **20**) and (*Z*)-1,5-octadien-3-one (no. **5**) (**Table 2**). Apart from these six substances, (*Z*)-3-hexenal, 1-octen-3-one, butanoic acid, and 2- and 3-methylbutanoic acid as well as 2-methoxyphenol were identified as further odor-active constituents in apricots, but with somewhat lower FD factors.

The results of the entire identification experiments are summarized in **Table 2**. Of the 26 compounds with FD factors between 8 and 2048, 22 odorants could be identified. Seven of them, namely, (*Z*)-3-hexenal, 1-octen-3-one, (*Z*)-1,5-octadien-3-one, 3-methyl-2,4-nonandione, 2-methoxyphenol, *trans*-4,5-epoxy-(*E*)-2-decenal, and eugenol, are reported here for the first time as constituents of fresh apricot.

Analysis of the chiral constituents on a special stationary phase revealed that linalool and γ-octalactone occurred as mixtures of the (*R*)- and (*S*)-isomers in ratios of 50.7:49.3 and 85.4:14.6, respectively. As far as γ-decalactone and γ-dodecalactone are concerned, only the (*R*)-isomer was present. These findings are in agreement with studies of Guichard et al. (*32*), who investigated the enantiomeric distribution of γ-lactone isomers in six apricot cultivars and also found a considerable excess of the (*R*)-isomer for all lactones investigated. By contrast, no studies exist so far on the enantiomeric distribution of (*R*)- and (*S*)-linalool in apricots.

The results of the AEDA suggested that γ-decalactone, (*E*)-β-damascenone, linalool, and δ-decalactone might be of special importance for the aroma of apricot. However, whereas most literature studies on apricot aroma are consistent in their findings in that γ-decalactone, linalool, and, to a somewhat smaller degree, δ-decalactone are important contributors to the overall aroma of apricot, no literature data previously existed pointing to a similar importance of (*E*)-β-damascenone. On the other hand, β-ionone, with a rather low FD factor (**Table 2**), was considered as an essential constituent of apricot aroma (*7*), whereas some other compounds with high FD factors, such as (*Z*)-1,5-octadien-3-one or 1-octen-3-one, were not characterized in previous studies. Like (*E*)-β-damascenone, these compounds showed high odor activities, but did not produce an FID signal and, therefore, might have been overlooked in investigations

Table 3. Concentrations of 31 Important Aroma Compounds in Fresh Apricots (Listed in Decreasing Concentration)

aroma compound	concn (μg/kg)	n^a	range (μg/kg)
acetic acid	8780	4	8190–9410
acetaldehyde	3560	2	3540–3580
γ-decalactone	509	6	407–561
pentanoic acid	267	2	262–272
δ-decalactone	245	6	210–269
linalool	183	6	136–218
γ-dodecalactone	181	6	146–215
2- and 3-methylbutanoic acid	160	4	147–170
hexanal	146	4	136–154
hexyl acetate	114	4	100–126
β-ionone	61.6	4	56.3–67.5
hexanoic acid	58.3	2	56.2–60.4
butanoic acid	50.6	4	42.9–60.0
(*E*)-2-hexenal	39.6	6	32.4–48.1
geraniol	35.2	3	32.9–39.4
γ-octalactone	27.4	5	20.0–37.9
(*Z*)-3-hexenal	10.2	3	9.5–11.0
(*E*,*Z*)-2,6-nonadienal	5.7	4	5.1–6.1
(*Z*)-3-hexenyl acetate	5.0	6	3.6–7.8
γ-nonalactone	2.7	3	2.6–2.8
1-octen-3-one	2.2	4	1.9–2.6
(*E*)-2-octenal	1.4	2	1.3–1.5
trans-4,5-epoxy-(*E*)-2-decenal	1.2	2	1.1–1.2
γ-undecalactone	1.0	4	0.9–1.2
eugenol	1.0	2	0.9–1.1
(*E*)-2-nonenal	0.7	3	0.6–0.7
(*E*)-β-damascenone	0.7	3	0.5–1.0
2-methoxyphenol	0.4	2	0.3–0.4
(*Z*)-1,5-octadien-3-one	0.3	4	0.2–0.3
3-methyl-2,4-nonandione	0.3	2	0.2–0.3

[a] Number of different fruits analyzed.

Table 4. Orthonasal Odor Thresholds (OOT) and Odor Activity Values (OAV) of Apricot Aroma Compounds

aroma compound	OOT (μg/L in water)	ref	OAV
β-ionone	0.20	*a*	308
(*Z*)-1,5-octadien-3-one	0.0012	*35*	250
γ-decalactone	2.6	*a*	196
(*E*,*Z*)-2,6-nonadienal	0.03	*11*	190
linalool	0.60[b]	*11*	155
acetaldehyde	25	*25*	142
γ-dodecalactone	2.0	*a*	91
hexyl acetate	2.0	*36*	57
1-octen-3-one	0.04	*a*	55
(*Z*)-3-hexenal	0.25	*37*	41
3-methyl-2,4-nonandione	0.01	*11*	30
hexanal	10	*a*	15
geraniol	3.2	*11*	11
trans-4,5-epoxy-(*E*)-2-decenal	0.12	*38*	10
δ-decalactone	51	*a*	4.8
(*E*)-β-damascenone	0.43	*a*	1.6
γ-octalactone	24	*a*	1.1
(*E*)-2-nonenal	0.69	*a*	1.0
acetic acid[c]	180000	*a*	<1
pentanoic acid[c]	24	*a*	<1
3-methylbutanoic acid[c]	1200	*a*	<1
hexanoic acid[c]	890	*11*	<1
butanoic acid[c]	7700	*a*	<1
(*E*)-2-hexenal	190	*a*	<1
(*Z*)-3-hexenyl acetate	8.0	*39*	<1
γ-nonalactone	27	*a*	<1
(*E*)-2-octenal	4.0	*36*	<1
γ-undecalactone	4.2	*a*	<1
eugenol	6.0	*40*	<1
2-methoxyphenol	2.5	*24*	<1

[a] Odor thresholds were determined by a group of 30 panelists at the German Research Center for Food Chemistry (Czerny et al., 2007; unpublished data). [b] The OAV of linalool was determined using the amount of (*R*)-linalool (50.7%) and the odor threshold of (*R*)-linalool (0.60 μg/L) for calculation. The amount of (*S*)-linalool, the odor threshold of which is about 80 times higher than that of the (*R*)-isomer (*41*), was neglected. [c] The odor threshold was determined at pH 4.5.

on apricot aroma performed without the application of GC-O. However, also the different cultivars used in previous studies or fruits of different ripening stages might be an explanation for these differences.

Quantitation of Aroma Compounds; Calculation of OAVs. The application of dilution to odor threshold techniques, such as the AEDA, does not provide immediate information about the contribution of single odorants to the overall aroma. The reason is that each volatile is completely vaporized during AEDA, so that this method is based on odor thresholds in air. Moreover, possible losses of odorants during the workup procedure are not fully taken into account. Therefore, to investigate the contribution of individual compounds to apricot aroma, 30 odorants were quantified in the fresh fruit purée by means of SIDAs.

The highest concentrations of 8.8 or 3.6 mg/kg, respectively, were determined for acetic acid and acetaldehyde, followed by γ-decalactone, pentanoic acid, δ-decalactone, linalool, γ-dodecalactone, 2- and 3-methylbutanoic acid, hexanal, and hexyl acetate (**Table 3**). Whereas these 11 compounds were present in concentrations >100 μg/kg, very low concentrations (<1 μg/kg) were found for (*E*)-2-nonenal, (*E*)-β-damascenone, 2-methoxyphenol, and 3-methyl-2,4-nonandione.

An important challenge in the analysis of fruit aroma compounds is fruit-to-fruit variations due to, for example, the different ripening stages. To address this problem, two to six different extracts, prepared in separate experiments from the same batch of fruits, were analyzed for the 30 compounds. Although the concentrations varied among the fruits analyzed (**Table 3**), for most odorants the differences amounted to about 30%, and only for (*Z*)-3-hexenyl acetate and γ-octalactone was a larger variation observed.

To correlate the quantitative data with the aroma of the food itself, the odor activity values (OAV = ratio of concentration to odor threshold) of the 30 compounds were calculated on the basis of odor threshold determined in water (*35*). Although it is known that the odor thresholds might be influenced by nonvolatile fruit compounds, water is the main constituent of apricots. The odor threshold of γ-undecalactone was determined for the first time in this study (cf. **Table 4**). The highest OAV was calculated for β-ionone (308), followed by (*Z*)-1,5-octadien-3-one (250) and γ-decalactone (196; **Table 4**). Surprisingly, (*E*,*Z*)-2,6-nonadienal, which did not show a very high FD factor, reached a high OAV of 190. Also, for 1-octen-3-one, an OAV of 55 was calculated. This is all the more remarkable because the odor qualities of (*Z*)-1,5-octadien-3-one (geranium-like), (*E*,*Z*)-2,6-nonadienal (cucumber-like), and 1-octen-3-one (mushroom-like) were not detectable in the overall aroma profile. Further compounds with high OAVs were linalool (155), acetaldehyde (142), γ-dodecalactone (91), hexyl acetate (57), and (*Z*)-3-hexenal (41). However, it is interesting to note that 12 compounds assigned as odor-active on the basis of AEDA results (**Table 2**), among them all acids and γ-nonalactone as well as γ-undecalactone, showed OAVs below 1 and should, consequently, not contribute significantly to apricot aroma.

The reason for the differences between FD factors and OAVs is simply that the entire amount of the odorants present in the aroma extract is vaporized during GC−olfactometry, whereas OAVs are calculated using odor thresholds in a matrix, thus considering only the amount of an individual odorant present

in the headspace above the matrix. Usually polar compounds are overestimated by AEDA, because they are quite soluble in water and, thus, their vapor pressure is comparatively low.

As already mentioned, all previous studies have considered γ-decalactone as the key aroma compound of apricot, and this lactone is suggested to be responsible for the typical sweet and fruity sensory properties of this fruit. Our results confirmed the importance of γ-decalactone in apricot aroma, because the lactone showed the third highest OAV of all compounds. However, although most studies discussed the additional importance of γ-decalactone, comparatively little attention has been paid to γ-dodecalactone, which has quite the same sensory properties. The present study shows that γ-dodecalactone, which is no. 7 in rank of the list of apricot volatiles sorted by their OAV (**Table 4**), is of higher importance than, for example, δ-nona-, δ-deca-, and δ-undecalactone. Obviously, in certain varieties this lactone is of greater importance for apricot aroma than previously assumed.

Although it can be suggested that the sweet, fruity aroma of apricot is mostly created by lactones and not by esters as is the case with other fruits, such as pineapple or banana, our data show that lactones are not entirely responsible for the typical apricot flavor. Although it has to be taken into account that the OAVs were calculated on the basis of odor thresholds in water, the very high OAVs of 301 and 155 determined for β-ionone and linalool, respectively, clearly show that also the metabolism of terpenes has a significant influence on the apricot aroma.

Until now, no studies exist reporting (*Z*)-1,5-octadien-3-one, (*E*,*Z*)-2,6-nonadienal, *trans*-4,5-epoxy-(*E*)-2-decenal, and 1-octen-3-one as volatile constituents of apricot. It can be assumed that these aldehydes or ketones, respectively, are formed in the fruit by an enzymatic degradation of either linolenic or linoleic acid. (*E*,*Z*)-2,6-Nonadienal is known to be formed from 9-hydroperoxy-10,12,15-octadecatrienoic acid (*42*), whereas (*Z*)-1,5-octadien-3-one and 1-octene-3-one are formed from linolenic or linoleic acid, respectively, via the 10-hydroperoxide (*14*). Furthermore, acetaldehyde, which had been neglected in most previous studies, is suggested as an important contributor to apricot flavor based on its high OAV. It makes an impression of freshness to the rather sweet, creamy odor note of the lactones and might, therefore, be essential for apricot aroma.

Aroma Reconstitution Experiments. In most cases, none of the odor-active compounds present in a food bear the typical aroma of the food itself. In a certain number of studies (e.g., refs *7*, *10*, *15*, *17*, *19*, *20*, and *23*), our group has been able to show that food aromas can be mimicked by a mixture of key odorants in their natural concentrations. However, as previously shown by us, for example, for the aroma of butter, in mixtures containing more than three odorants their typical odor notes can no longer be singly perceived (*17*). Because it is difficult to predict the overall aroma of a complex mixture of compounds, aroma reconstitution experiments are a useful tool to verify the correctness of the quantitative data. For this purpose, all 18 aroma compounds with OAVs $\geq$ 1 (**Table 4**) were mixed in the same concentrations as they occur in the fruits using pure reference compounds. Differences or similarities were then determined by comparing the odor of the model mixture with the original fruit puree. The results of this experiment are illustrated in **Figure 1**. The aroma profiles of the fresh fruit and that of the recombinate 1 showed a good agreement apart from some differences in the fruity/fresh, green/grassy, and flowery/citrus-like odor notes, which were perceived a bit more intensely in the apricots. The overall similarity between the fruits and the recombinate was marked 2.6 on a scale from 0 to 3.

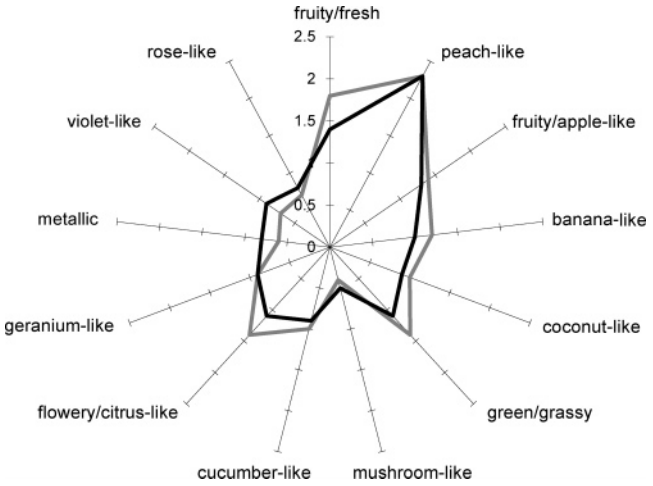

Figure 1. Aroma profile analysis of apricots (—) and the aroma recombinate (**—**).

These data suggest that the key aroma compounds of apricot were successfully identified in this study.

Omission Experiment. Apricots contain a number of aroma compounds, which are products of an enzymatic lipid peroxidation. Although some of them, namely, (*Z*)-1,5-octadien-3-one, (*E*,*Z*)-2,6-nonadienal, and 1-octen-3-one, have rather high OAVs, others [e.g., *trans*-4,5-epoxy-(*E*)-2-decenal and (*E*)-2-nonenal] were of somewhat lower importance. What they have in common, though, is that their odor qualities (geranium-like, cucumber-like, mushroom-like, metallic, and fatty-cucumber-like) seem to be quite unusual for the apricot aroma. To find out whether these compounds are of any greater importance in apricot aroma, a recombinate containing all aroma compounds with OAVs $\geq$ 1, except (*Z*)-1,5-octadien-3-one, (*E*,*Z*)-2,6-nonadienal, 1-octen-3-one, *trans*-4,5-epoxy-(*E*)-2-decenal, and (*E*)-2-nonenal, was prepared and presented to the sensory panel in a triangle test in comparison with the original recombinate. The omission of the five aroma compounds turned out to be highly significant, because the deviating sample was recognized by 23 of 32 panelists. Most panelists confirmed that the original recombinate was closer to the aroma of fresh apricots than the sample in which the lipid peroxidation products were omitted.

In summary, the results show that the responses of the human odorant receptors toward apricot aroma can be closely mimicked by a mixture of 18 volatiles being identical in their concentrations to those present in the fruit. Interestingly, also compounds with odor qualities not resembling fruity notes, such as (*Z*)-1,5-octadien-3-one, are also needed as aroma constituents. The data confirm again that odor-active components in a complex aroma profile can be elucidated using approaches of molecular sensory science. The set of such key odorants can be assigned as "blueprint" of a mixture interacting with the human odorant receptors and finally evoking the overall odor perception in the brain.

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