

# 5 Aroma Compounds

## 5.1 Foreword

### 5.1.1 Concept Delineation

When food is consumed, the interaction of taste, odor and textural feeling provides an overall sensation which is best defined by the English word “flavor”. German and some other languages do not have an adequate expression for such a broad and comprehensive term. Flavor results from compounds that are divided into two broad classes: Those *responsible for taste* and those *responsible for odors*, the latter often designated as aroma substances. However, there are compounds which provide both sensations.

Compounds *responsible for taste* are generally nonvolatile at room temperature. Therefore, they interact only with taste receptors located in the taste buds of the tongue. The four important basic taste perceptions are provided by: sour, sweet, bitter and salty compounds. They are covered in separate sections (cf., for example, 8.10, 22.3, 1.2.6, 1.3.3, 4.2.3 and 8.8). Glutamate stimulates the fifth basic taste (cf. 8.6.1).

*Aroma substances* are volatile compounds which are perceived by the odor receptor sites of the smell organ, i. e. the olfactory tissue of the nasal cavity. They reach the receptors when drawn in through the nose (orthonasal detection) and via the throat after being released by chewing (retronasal detection). The concept of aroma substances, like the concept of taste substances, should be used loosely, since a compound might contribute to the typical odor or taste of one food, while in another food it might cause a faulty odor or taste, or both, resulting in an off-flavor.

### 5.1.2 Impact Compounds of Natural Aromas

The amount of volatile substances present in food is extremely low (ca. 10–15 mg/kg). In general, however, they comprise a large number of

components. Especially foods made by thermal processes, alone (e. g., coffee) or in combination with a fermentation process (e. g., bread, beer, cocoa, or tea), contain more than 800 volatile compounds. A great variety of compounds is often present in fruits and vegetables as well.

All the known volatile compounds are classified according to the food and the class of compounds and published in a tabular compilation (*Nijssen, L. M. et al., 1999*). A total of 7100 compounds in more than 450 foods are listed in the 1999 edition, which is also available as a database on the internet.

Of all the volatile compounds, only a limited number are important for aroma. Compounds that are considered as aroma substances are prima-

**Table 5.1.** Examples of key odorants

Compound	Aroma	Occurrence
(R)-Limonene	Citrus-like	Orange juice
(R)-1-p-Menthene-8-thiol	Grapefruit-like	Grapefruit juice
Benzaldehyde	Bitter almond-like	Almonds, cherries, plums
Neral/geranial	Lemon-like	Lemons
1-(p-Hydroxyphenyl)-3-butanone (raspberry ketone)	Raspberry-like	Raspberries
(R)-(-)-1-Octen-3-ol	Mushroom-like	Champignons, Camembert cheese
(E,Z)-2,6-Nonadienal	Cucumber-like	Cucumbers
Geosmin	Earthy	Beetroot
trans-5-Methyl-2-hepten-4-one (filbertone)	Nut-like	Hazelnuts
2-Furfurylthiol	Roasted	Coffee
4-Hydroxy-2,5-dimethyl-3(2H)-furanone	Caramel-like	Biscuits, dark beer, coffee
2-Acetyl-1-pyrroline	Roasted	White-bread crust

rily those which are present in food in concentrations higher than the odor and/or taste thresholds (cf. "Aroma Value", 5.1.4). Compounds with concentrations lower than the odor and/or taste thresholds also contribute to aroma when mixtures of them exceed these thresholds (for examples of additive effects, see 3.2.1.1, 20.1.7.8, 21.1.3.4).

Among the aroma substances, special attention is paid to those compounds that provide the characteristic aroma of the food and are, consequently, called key odorants (character impact aroma compounds). Examples are given in Table 5.1.

In the case of important foods, the differentiation between odorants and the remaining volatile compounds has greatly progressed. Important findings are presented in the section on "Aroma" in the corresponding chapters.

### 5.1.3 Threshold Value

The lowest concentration of a compound that is just enough for the recognition of its odor is called the odor threshold (recognition threshold). The detection threshold is lower, i. e., the concentration at which the compound is detectable but the aroma quality still cannot be unambiguously established. The threshold values are frequently determined by smelling (orthonasal value) and by tasting the sample (retronasal value). With a few exceptions, only the orthonasal values are given in this chapter. Indeed, the example of the carbonyl compounds shows how large the difference between the ortho- and retronasal thresholds can be (cf. 3.7.2.1.9).

Threshold concentration data allow comparison of the intensity or potency of odorous substances. The examples in Table 5.2 illustrate that great differences exist between individual aroma compounds, with an odor potency range of several orders of magnitude.

In an example provided by nootkatone, an essential aroma compound of grapefruit peel oil (cf. 18.1.2.6.3), it is obvious that the two enantiomers (optical isomers) differ significantly in their aroma intensity (cf. 5.2.5 and 5.3.2.4) and, occasionally, in aroma quality or character.

The threshold concentrations (values) for aroma compounds are dependent on their vapor pressure, which is affected by both temperature and

**Table 5.2.** Odor threshold values in water of some aroma compounds (20 °C)

Compound	Threshold value (mg/l)
Ethanol	100
Maltol	9
Furfural	3.0
Hexanol	2.5
Benzaldehyde	0.35
Vanillin	0.02
Raspberry ketone	0.01
Limonene	0.01
Linalool	0.006
Hexanal	0.0045
2-Phenylethanal	0.004
Methylpropanal	0.001
Ethylbutyrate	0.001
(+)-Nootkatone	0.001
(-)-Nootkatone	1.0
Filbertone	0.00005
Methylthiol	0.00002
2-Isobutyl-3-methoxypyrazine	0.000002
1-p-Menthene-8-thiol	0.0000002

medium. Interactions with other odor-producing substances can result in a strong increase in the odor thresholds. The magnitude of this effect is demonstrated in a model experiment in which the odor thresholds of compounds in water were determined in the presence and absence of 4-hydroxy-2,5-dimethyl-3(2H)-furanone (HD3F). The results in Table 5.3 show that HD3F does not influence the threshold value of 4-vinylguaiacol. However, the threshold values of the other odor-

**Table 5.3.** Influence of 4-hydroxy-2,5-dimethyl-3(2H)-furanone (HD3F) on the odor threshold of aroma substances in water

Compound	Threshold value ( $\mu\text{g}/\text{l}$ )		Ratio II to I
	I <sup>a</sup>	II <sup>b</sup>	
4-Vinylguaiacol	100	90	$\approx 1$
2,3-Butanedione	15	105	7
2,3-Pentanedione	30	150	5
2-Furfurylthiol	0.012	0.25	20
$\beta$ -Damascenone	$2 \times 10^{-3}$	0.18	90

<sup>a</sup> I, odor threshold of the compound in water.

<sup>b</sup> II, odor threshold of the compound in an aqueous HD3F solution having a concentration (6.75 mg/l, aroma value A = 115) as high as in a coffee drink.

**Table 5.4.** Comparison of threshold values<sup>a</sup> in water and beer

Compound	Threshold (mg/kg) in	
	Water	Beer
n-Butanol	0.5	200
3-Methylbutanol	0.25	70
Dimethylsulfide	0.00033	0.05
(E)-2-Nonenal	0.00008	0.00011

<sup>a</sup> Odor and taste.

ants increase in the presence of HD3F. This effect is the greatest in the case of  $\beta$ -damascenone, the threshold value being increased by a factor of 90. Other examples in this book which show that the odor threshold of a compound increases when it is influenced by other odor-producing substances are a comparison of the threshold values in water and beer (cf. Table 5.4) as well as in water and in aqueous ethanol (cf. 20.2.6.9).

### 5.1.4 Aroma Value

As already indicated, compounds with high “aroma values” may contribute to the aroma of foods. The “aroma value”  $A_x$  of a compound is calculated according to the definition:

$$A_x = \frac{c_x}{a_x} \quad (5.1)$$

( $c_x$ : concentration of compound X in the food,  $a_x$ : odor threshold (cf. 5.1.3) of compound X in the food). Methods for the identification of the corresponding compounds are described under Section 5.2.2.

The evaluation of volatile compounds on the basis of the aroma value provides only a rough pattern at first. The dependence of the odor intensity on the concentration must also be taken into account. In accordance with the universally valid law of *Stevens* for physiological stimuli, it is formulated as follows:

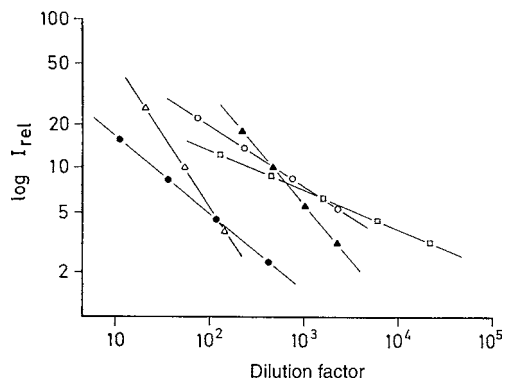
$$E = k \cdot (S - S_0)^n \quad (5.2)$$

$E$ : perception intensity,  $k$ : constant,  $S$ : concentration of stimulant,  $S_0$ : threshold concentration of stimulant.

The examples presented in Fig. 5.1 show that the exponent  $n$  and, therefore, the dependency of the odor intensity on the concentration can vary substantially. Within a class of compounds, the range of variations is not very large, e. g.,  $n = 0.50$ – $0.63$  for the alkanals  $C_4$ – $C_9$ .

In addition, additive effects that are difficult to assess must also be considered. Examinations of mixtures have provided preliminary information. They show that although the intensities of compounds with a similar aroma note add up, the intensity of the mixture is usually lower than the sum of the individual intensities (cf. 3.2.1.1). For substances which clearly differ in their aroma note, however, the odor profile of a mixture is composed of the odor profiles of the components added together, only when the odor intensities are approximately equal. If the concentration ratio is such that the odor intensity of one component predominates, this component then largely or completely determines the odor profile.

Examples are (E)-2-hexenal and (E)-2-decenal which have clearly different odor profiles (cf. Fig. 5.2 a and 5.2 f). If the ratio of the odor intensities is approximately one, the odor notes of both aldehydes can be recognized in the odor profile of the mixture (Fig. 5.2 d). But if the dominating odor intensity is that of the decenal (Fig. 5.2 b), or of the hexenal (Fig. 5.2 e), that particular note determines the odor profile of the mixture.

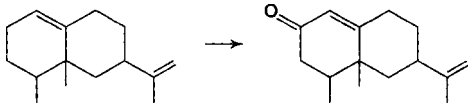
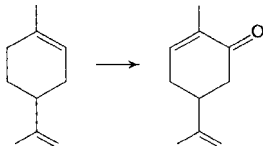
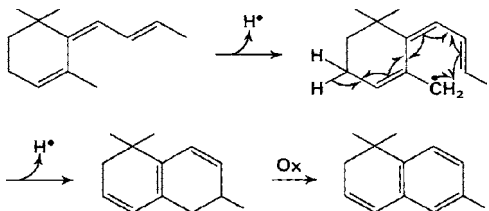


**Fig. 5.1.** Relative odor intensity  $I_{rel}$  (reference: n-butanol) as a function of the stimulant concentration (according to *Dravnieks*, 1977).

Air saturated with aroma substance was diluted. ●—●—●  $\alpha$ -pinene, ○—○—○ 3-methylbutyric acid methyl ester,  $\Delta$ — $\Delta$ — $\Delta$  hexanoic acid,  $\blacklozenge$ — $\blacklozenge$ — $\blacklozenge$  2,4-hexadienal,  $\square$ — $\square$ — $\square$  hexylamine



**Table 5.5.** “Off-flavors” in food products

Food product	Off-flavor	Cause
Milk	Sunlight flavor	Photooxidation of methionine to methional (with riboflavin as a sensitizer)
Milk powder	Bean-like	The level of O <sub>3</sub> in air too high: ozonolysis of 8,15- and 9,15-isolinoleic acid to 6-trans-nonenal
Milk powder	Gluey	Degradation of tryptophan to o-amino-acetophenone
Milk fat	Metallic	Autoxidation of pentaene- and hexaene fatty acids to octa-1,cis-5-dien-3-one
Milk products	Malty	Faulty fermentation by <i>Streptococcus lactis</i> , var: <i>maligenes</i> ; formation of phenylacetaldehyde and 2-phenylethanol from phenylalanine
Peas, deep froze	Hay-like	Saturated and unsaturated aldehydes, octa-3,5-dien-2-one, 3-alkyl-2-methoxypyrazines, hexanal
Orange juice	Grapefruit note	Metal-catalyzed oxidation or photooxidation of valencene to nootkatone
		
Orange juice	Terpene note	d-Limonene oxidation to carvone
		
Passion fruit juice	Aroma flattening during pasteurization	Oxidation of (6-trans-2'-trans)-6-(but-2'-enyliden)-1,5,5-trimethylcyclohex-1-ene to 1,1,6-trimethyl-1,2-dihydronaphthalene:
		
Beer	Sunlight flavor	Photolysis of humulone: reaction of one degradation product with hydrogen sulfide yielding 3-methyl-2-buten-1-thiol
Beer	Phenolic note	Faulty fermentation: hydrocinnamic acid decarboxylation by <i>Hafnia protea</i>

