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Relationships between temporal release of aroma compounds in a model mouth system and their physico-chemical characteristics

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Abstract

The influence of matrix composition and mastication on the temporal release of seven aroma compounds was studied in a model mouth system. 2-Butanone, diacetyl, ethyl acetate, 3-methyl-1-butanol, hexanal, 2-heptanone and ethyl butyrate were released from water and sunflower oil, with and without mastication, for 15, 30, 60, 120, 240, 480 and 720 s. Aroma compounds were quantified by gas chromatography/mass spectrometry. Volatile compounds were released at significantly different rates. The release of hydrophobic compounds from the oil was decreased, whereas the release of the hydrophilic compound diacetyl was increased in comparison with the water matrix. Interactions were observed between volatile compounds and matrix, as well as between volatile compounds and mastication. Linear release rate constants were related to physico-chemical characteristics, such as molecular weight, boiling points, vapour pressures, octanol–water, gas–water and gas–oil partition coefficients. The octanol–water partition coefficients correlated reasonably well with linear release rate constants for the release from water and oil without mastication, and from water with mastication. The other physico-chemical characteristics correlated poorly with linear release rate constants. © 2000 Elsevier Science Ltd. All rights reserved.

1. Introduction

Aroma release is a critical factor governing aroma perception. Perception of aroma during eating is determined by those compounds available to the sensory system as a function of time (Taylor, 1998). The aroma stimulus depends upon the concentration of aroma compounds in the nasopharynx, which in turn, is affected by release rates of the compounds from the food in the mouth. Food composition affects aroma release as aroma compounds may be dissolved, adsorbed, bound, entrapped, encapsulated or diffusion-limited by food components. The relative importance of each of these mechanisms with respect to aroma release varies with the properties of the aroma compounds and the physical and chemical properties of the components in the food (Kinsella, 1988).

Lipids dissolve and absorb most organic aroma compounds and greatly affect their perception. Aroma compounds partition according to their physical properties between product and gas phases. Their generally hydrophobic nature leads to concentration in the lipid phase. This greatly reduces their partitioning into gas or aqueous phases and markedly increases flavour threshold concentrations (Buttery, Guadagni & Ling, 1973; Forss, 1969; Guyot, Bonnafont, Lesschaeve, Issanchou, Voilley & Spinnler, 1996).

Headspace analysis has been widely used to determine factors affecting partitioning of volatiles between product and gas phase. In a near ideal state of infinite dilution, Henry's law prevails and, at equilibrium, the partial pressure of the volatile in the gas phase above the solution is proportional to the volatile concentration in the liquid phase of the food. Under these conditions, the partition coefficient is defined as the ratio of the concentration of the volatile in the gas phase to its concentration in the liquid phase (Taylor, 1998).

Partition coefficients provide information on flavour–matrix interactions under equilibrium conditions. However, during the eating process, equilibrium is not achieved in the mouth. Evaluation of the behaviour of aroma compounds in model food systems facilitates the reconstruction of the interactions between the volatile compounds and food components in complex food systems. Methods have been developed to measure volatile release from simple or more complicated food systems in relation to physico-chemical parameters of (model)

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foods and aroma compounds. Roberts and Acree (1996a) developed a system simulating mouth conditions, i.e. the Retronasal Aroma Simulator. In this large-scale blender system, release of volatiles is measured under defined conditions. They studied temperature and viscosity effects on release of a range of compounds with various physico-chemical properties. The present authors presented their model mouth system first in 1994 (van Ruth, Roozen & Cozijnsen, 1994). This system has a similar volume as the human mouth, is temperature controlled, and allows salivation and mastication to be applied. Release of aroma compounds from complicated food systems, such as various rehydrated vegetables, bulk oils, emulsions and dressings, have been studied in this model system (van Ruth & Roozen, 2000; Odake, Roozen & Burger, 1998; van Ruth, Roozen, Nahon, Cozijnsen & Posthumus, 1996). These studies focused on the effects of saliva composition, saliva volume, mastication and food composition on the release of volatile compounds. Aroma release as a function of time (temporal release) has not been studied in this model mouth system so far. However, with the help of rapid gas-phase analysis techniques, such as Tenax trapping (Delahunty, Piggott, Conner & Paterson, 1996; Roozen & Legger-Huysman, 1994) and direct mass spectrometry methods (Taylor & Linforth, 1997), measurements at the time-scale of eating can be executed.

The aim of the present study was to investigate temporal release of seven aroma compounds from an oil or water matrix in a model mouth system, as well as the influence of mastication. Differences in temporal release of the aroma compounds were related to the physico-chemical characteristics of the compounds.

2. Materials and methods

2.1. Materials

Seven aroma compounds: 2-butanone, diacetyl, ethyl acetate, 3-methyl-1-butanol, hexanal, 2-heptanone and ethyl butyrate (suppliers: Table 1) were dissolved in distilled water and in sunflower oil (cold pressed sunflower oil; Suma Wholefoods, Dean Clough, Hailfax, UK) in 22 ml vials in quadruplicate (0.1% v/v for each compound). The samples were incubated for 24 h at 4°C to ensure even distribution prior to analysis. Molecular weights, boiling points and odour descriptors of the compounds are presented in Table 1. Control samples of oil and water without added compounds were incubated and analysed to assure that neither formation of volatile compounds, nor impurities interfered with the release data and static headspace data.

2.2. Methods

2.2.1. Release of aroma compounds in the model mouth system

Aroma compounds were isolated in a model mouth system, the latest version of which has been reported by van Ruth and Roozen (2000). The oil or water aroma mixtures (20 ml) were transferred into the sample flask (70 ml, 37°C) of the model mouth system. The headspace was flushed with purified nitrogen gas (100 ml min^{-1}). The released volatile compounds were trapped in Tenax (Tenax TA 60/80; Supelco, Bellefonte, PA, USA) for 15, 30, 60, 120, 240, 480 and 720 s. Isolation of the volatile compounds was carried out with and without a plunger making up-and-down screwing movements to simulate mastication. Isolation of volatile compounds was carried out for each incubated oil and water sample (including control samples), with and without mastication. Volatile compounds were analysed by gas chromatography/mass spectrometry, as described in Section 2.2.3.

2.2.2. Determination of equilibrium headspace concentrations by static headspace analysis

The oil and water mixtures (0.1% v/v for each compound, 5 ml) were transferred into 22 ml vials. Samples were equilibrated in a waterbath at 37°C for 2.5 h. Preliminary experiments showed no increase in headspace

Table 1
Aroma compounds used in temporal release experiments, molecular weights (M_w), boiling points (Bp), odour descriptors and suppliers

Number	Compound	M_w	Bp (°C)	Odour descriptor[a]	Supplier
1	2-Butanone	72	80	Ethereal	Aldrich[c]
2	Diacetyl	86	88	Buttery	Merck[b]
3	Ethyl acetate	88	77	Ethereal-fruity	Sigma[c]
4	3-Methyl-1-butanol	88	131	Alcoholic, fruity-winey	Lancaster[d]
5	Hexanal	100	128	Fatty-green, grassy	Aldrich
7	2-Heptanone	114	151	Fruity-spicy	Aldrich
6	Ethyl butyrate	116	122	Ethereal-fruity	Merck

[a] Arctander (1969).
[b] Merck, Hohenbrunn, Munich, Germany.
[c] Aldrich, Steinheim, Germany.
[d] Lancaster, Walkerburn, UK.

concentrations after 2 h equilibration. The headspace (5 ml) was injected on Tenax TA and aroma compounds were analysed by gas chromatography/mass spectrometry, as described in Section 2.2.3. Four replicates of both oil and water mixtures were analysed (one analysis per equilibrated vial), as well as control samples. Concentrations in the headspace of the samples were calculated and divided by the concentrations in the liquid phase for determination of the gas/liquid partition coefficients of the compounds in the two matrices.

2.2.3. *Gas chromatography/mass spectrometry analysis of volatile compounds*

The aroma compounds, trapped on Tenax TA, were identified and quantified by combined gas chromatography (GC) (Varian Star 3400 CX, JVA Analytical Ltd, Dublin, Ireland) and mass spectrometry (MS; Varian Saturn 3, JVA Analytical Ltd, Dublin, Ireland). Desorption of volatile compounds from Tenax (220°C, 4 min) was performed by a thermal desorption device (Tekmar Purge and Trap 3000 concentrator, JVA Analytical Ltd, Dublin, Ireland). Through a heated transfer line, the compounds were directed to the GC column (Rtx®−502.2 capillary column, 60 m length, 0.53 mm id, film thickness 3.0 μm; Interscience, Belfast, Northern Ireland). An initial oven temperature of 40°C was used for 3 min, followed by a rate increase of 2°C min^{-1} to 80°C, then by 3°C min^{-1} to 200°C and finally by 10°C min^{-1} to 220°C, with a final hold at 220°C for 2 min. Mass spectra were obtained with 70 eV electron impact ionisation, while the mass spectrometer was continuously scanning from m/z 40 to 400 at a scan speed of 3 scans s^{-1}. Volatile compounds were identified by comparison of their spectra with bibliographic data, and by comparison with spectra and retention times of single authentic compounds. Seven concentrations of volatile compounds in pentane were analysed in triplicate for calibration, allowing quantification of compounds isolated in the model mouth and in the static headspace system.

2.2.4. *Calculation of linear release rate constants*

The collection of aroma compounds in the model mouth system on seven Tenax traps over 720 s showed the dynamics of release. Linear release rate constants (k) were estimated from the rate of adsorption on the traps according to the method described by Roberts and Acree (1995).

$$k = (\mathrm{d}[A]/\mathrm{d}t)_{\mathrm{trap}}/[A_0]$$

where:

$[A]$ = concentration of volatile in liquid phase (g/l),
$[A_0]$ = initial concentration of volatile in liquid phase (g/l).
t = time in min.

As the amounts of aroma compounds collected on the traps were negligible compared to the amounts remaining in the liquid phase, the assumption can be made that the concentration of aroma compounds in the liquid phase during the collection of the volatiles is equal to the initial concentration. The linear rate constant (k) is defined as the linear release rate over time divided by the initial concentration.

2.2.5. *Statistical analysis*

The isolated amounts of aroma compounds for the various samples were subjected to analysis of variance to determine significant differences in release. The factors included the type of compound, the matrix, mastication and time interval. Significant differences between the linear release rate constants of all the compounds in the oil and water matrix were determined by sign tests. Spearman's ranked correlation tests were performed on linear release rate constants, boiling points, vapour pressures, octanol–water, gas–water and gas–oil partition coefficients of the compounds. A significance level of $P < 0.05$ was used throughout the study.

3. Results and discussion

3.1. *Release in the model mouth system*

Temporal aroma release of seven aroma compounds from a water matrix and an oil matrix was studied in the model mouth system. The aroma compounds selected are present in the volatile fraction of many foods as has been reported by numerous authors (Maarse, Visscher, Willemsen & Boelens, 1989). Odour descriptors vary among the compounds (Table 1). The compounds differed considerably in physico-chemical characteristics as well, such as molecular weight (Table 1), boiling points (Table 1), vapour pressures (Fig. 1) and octanol-water partition coefficients (Log P; Fig. 1). Vapour pressures and octanol–water partition coefficients can be considered measures for volatility and hydrophobicity, respectively.

The amounts of aroma compounds released over seven time intervals (15–720 s) were quantified by GC/MS and are presented for the water matrix in Table 2 and for the oil matrix in Table 3. Analysis of variance ($P < 0.05$) of the raw release data showed a significant effect of the type of compound. In addition, a significant interaction between the type of compound and mastication, as well as between the type of compound and the matrix was observed. Apparently, the amount released over the various time intervals depended on the type of compound. It was also affected by the matrix in which the compound was present and by mastication. Release of hydrophobic compounds (all except diacetyl) from the oil was reduced, while release of the hydrophilic

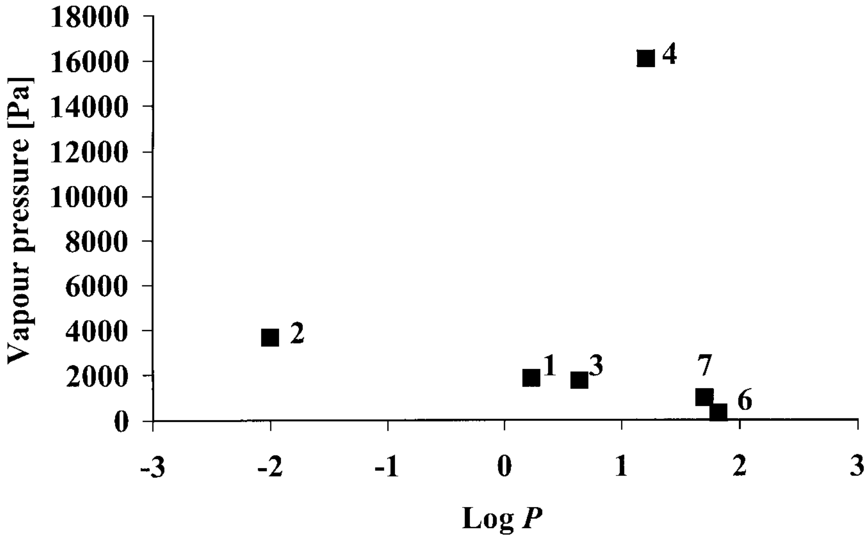

Fig. 1. Saturated vapour pressures at 25°C (Antoine equation; Reid, 1987) and octanol–water partition coefficients (Log *P*; Lide, 1997) of aroma compounds used in temporal release experiments. Numbers in the graph refer to compounds listed in Table 1. Vapour presssure of hexanal (No. 5) could not be calculated as constants were not available.

compound diacetyl from the oil was increased in comparison with the water matrix (Tables 2 and 3). Mastication showed a larger effect on the release from oil than from water.

Linear release rate constants (k) were calculated for the various samples (Table 4). Roberts and Acree (1996a) reported linear release constants for α-pinene, ethyl-2-methyl-butyrate, 1,8-cineole in their Retronasal Aroma Simulator, which were slightly higher than those in the present study. Constants of 2-methoxy-3-methylpyrazine, vanillin, butyric acid and maltol were in the same range as the values presented in Table 4. It is remarkable that, although different volatile compounds were studied, similar constants were found in both mouth simulators. The dimensions of the systems and shearing/mastication devices differ considerably.

The influence of the matrix varied for the various compounds, as indicated by the ratio k_{oil} to k_{water} (Table 4). The ratio decreased with increased molecular weight and hydrophobicity, which is the result of larger differences between the two matrices for the compounds with a higher molecular weight. The effect of the matrix on aroma release are in agreement with dynamic headspace studies of Salvador, Bakker, Langley, Potjewijd, Martin and Elmore (1994), which showed higher release rates for diacetyl from oil than from water. In addition, Druaux, Thanh, Seuvre and Voilley (1998) reported liquid–gas phase transfer rates for ethyl acetate, which

Table 2
Quantities of aroma compounds released from water (μg) for various time periods in a model mouth system, with and without mastication ($n = 4$)

Compound	Time period of aroma release (s)						
	15	30	60	120	240	480	720
Without mastication							
2-Butanone	2.86	3.36	6.22	12.94	14.36	20.98	31.11
Diacetyl	1.87	2.17	3.84	6.61	7.48	9.87	11.32
Ethyl acetate	9.54	10.66	21.00	42.06	47.71	63.17	67.72
3-Methyl-1-butanol	9.11	12.37	26.05	35.46	45.71	74.38	125.43
Hexanal	5.57	7.25	8.40	17.15	23.08	96.49	160.97
2-Heptanone	9.79	13.8	17.21	38.01	55.12	176.79	291.47
Ethyl butyrate	7.05	8.94	10.60	28.38	34.81	161.19	266.46
With mastication							
2-Butanone	0.49	0.67	1.01	3.52	16.00	28.70	35.44
Diacetyl	0.40	0.48	0.66	1.76	2.02	3.80	4.42
Ethyl acetate	0.70	1.32	2.05	9.80	50.88	108.80	136.29
3-Methyl-1-butanol	1.27	2.05	7.42	13.20	40.77	104.03	129.72
Hexanal	1.08	1.70	4.38	11.43	38.18	91.98	117.09
2-Heptanone	3.22	4.38	12.17	27.78	81.52	288.53	357.36
Ethyl butyrate	1.09	1.83	4.89	15.36	64.74	143.03	188.99

Table 3
Quantities of aroma compounds released from sunflower oil (μg) for various time periods in a model mouth system, with and without mastication ($n = 4$)

Compound	Time period of aroma release (s)						
	15	30	60	120	240	480	720
Without mastication							
2-Butanone	0.34	0.34	3.18	3.18	3.19	3.20	3.42
Diacetyl	3.56	4.77	11.32	11.46	44.82	87.77	101.00
Ethyl acetate	0.38	0.49	1.13	1.15	2.27	2.70	3.14
3-Methyl-1-butanol	0.0048	0.14	0.58	0.60	2.70	5.34	5.90
Hexanal	0.22	0.30	0.84	0.87	2.92	6.85	7.21
2-Heptanone	0.0021	0.19	1.16	1.33	4.39	5.05	6.22
Ethyl butyrate	0.49	0.65	1.47	1.52	3.32	7.87	8.13
With mastication							
2-Butanone	10.23	10.38	10.85	11.14	15.29	18.31	20.55
Diacetyl	0.80	0.92	1.27	1.55	3.51	4.09	4.75
Ethyl acetate	20.10	20.91	23.13	24.66	38.52	49.56	58.16
3-Methyl-1-butanol	9.76	11.08	15.03	17.33	26.86	36.55	42.68
Hexanal	2.85	3.13	4.21	4.87	8.06	11.41	13.77
2-Heptanone	3.46	3.97	5.42	6.47	9.43	12.85	15.58
Ethyl butyrate	4.31	4.80	6.35	7.36	12.27	17.54	20.67

were four times larger for water than for linoleic acid. The same trend was shown by Guyot et al. (1996) with respect to compound–matrix interactions in relation to odour perception. They reported higher odour intensities for hydrophobic compounds in water and more pronounced odours for hydrophilic compounds in oil.

The influence of the type of compound was mainly observed in the water matrix. Generally larger constants were observed for the hydrophobic compounds than for the smaller, more hydrophilic compounds. Similar conclusions could not be drawn for the relationship of hydrophilic/hydrophobic character of the compounds and release from the oil. Present results confirm studies of Roberts and Acree (1995). They found a reasonable correlation between the linear release rate for aroma release from water and the hydrophobic character of the compounds, which was not observed for the soybean oil matrix used in their experiments. Aroma release depends on partitioning and mass transfer factors (De Roos & Wolswinkel, 1994; Harrison, Hills, Bakker & Clothier, 1997; Marin, Baeck, & Taylor, 1999). The higher viscosity of the oil is likely to result in a larger mass transfer component than it is for the water matrix.

Relationships between viscosity, mass transfer coefficients and aroma release were presented recently by Nahon, Harrison and Roozen (2000), Harrison et al. (1997) and Roberts and Acree (1996b). The more pronounced influence of mass transfer is also indicated by the larger effect of mastication on the aroma release from the oil, in comparison with water. There is no overall significant effect of mastication in water (comparison of k_{water} with and without mastication, sign test, $P < 0.05$), but mastication resulted in significant increased linear release rate constants for the oil. The various compounds were differently affected by mastication, which resulted in altered proportions of the compounds

Table 4
Linear release rate constants $(k \times 10^{-5})$ and correlation coefficients (R^2) of aroma compounds released from water or sunflower oil in a model mouth system, with and without mastication

Compound	Without mastication					With mastication				
	Water		Oil		Ratio k_{oil} to k_{water}	Water		Oil		Ratio k_{oil} to k_{water}
	k_{water}	R^2	k_{oil}	R^2		k_{water}	R^2	k_{oil}	R^2	
2-Butanone	15	0.97	1	0.65	0.10	20	0.99	7	0.83	0.37
Diacetyl	4	0.92	46	0.98	10.68	2	0.97	2	0.94	1.02
Ethyl acetate	30	0.90	1	0.93	0.05	69	0.99	22	0.92	0.31
3-Methyl-1-butanol	58	0.99	3	0.98	0.06	72	0.99	19	0.95	0.27
Hexanal	78	0.98	4	0.97	0.05	63	0.99	6	0.97	0.10
2-Heptanone	144	0.99	3	0.95	0.02	197	0.99	7	0.95	0.03
Ethyl butyrate	124	0.98	4	0.97	0.03	96	0.99	9	0.96	0.09

Table 5
Equilibrium headspace concentrations (μg/ml headspace) of aroma compounds dissolved in water or sunflower oil at 37°C ($n = 4$)

Compound	Water	Oil	Ratio oil to water
2-Butanone	0.091	0.090	0.99
Diacetyl	0.055	0.065	1.18
Ethyl acetate	0.254	0.105	0.41
3-Methyl-1-butanol	0.083	0.030	0.36
Hexanal	0.327	0.020	0.06
2-Heptanone	0.487	–[a]	< 0.02
Ethyl butyrate	0.518	0.029	0.06

[a] Below detection.

released. These changed proportions might influence the overall aroma of the mixture.

3.2. Equilibrium headspace concentrations

Equilibrium headspace concentrations of the seven aroma compounds were determined at 37°C (Table 5) in order to study the partitioning aspect of aroma release. A higher headspace concentration of diacetyl was observed for the oil than for the water matrix (ratio > 1; Table 5). The other compounds showed higher headspace concentrations in water than in the oil (ratio < 1). The difference in headspace concentration between oil and water is more pronounced for the higher molecular weight compounds, which is reflected by the decreasing ratio with molecular weight. The ratio of the linear release rate constants 'k_{oil} to k_{water}' (Table 4) showed the same trend as the equilibrium headspace concentrations. However, as there is a mass transfer component involved in the release, the differences between oil and water are in the same direction but more distinct. Equilibrium headspace data are in agreement with the classical studies of Buttery et al. (1973) and Buttery, Ling and Guadagni (1969).

3.3. Comparison of release and physico-chemical characteristics of aroma compounds

Linear release rate constants of the seven aroma compounds in water and sunflower oil, with and without mastication (Table 4) were correlated with their physico-chemical characteristics (Table 6). These characteristics included molecular weights (Table 1), boiling points (Table 1), vapour pressures (Fig. 1), octanol–water partition coefficients (Fig. 1) gas–water and gas–oil partition coefficients (both based on data Table 5). Generally, the characteristics did not correlate very well with the release rate constants of the samples.

Focusing on the type of sample, all characteristics correlated more or less with aroma release from water without mastication, except for the vapour pressure. Mass transfer effects are expected to have limited influence under these conditions, therefore, aroma release is mainly determined by partitioning factors. The viscosity of the oil and mastication is likely to have resulted in an important effect of mass transfer, which explains the poor correlations for the oil samples and the mastication samples between linear release rates and characteristics which are more or less related to partitioning of compounds over liquid and gas phase.

When focusing on the characteristics which predict aroma release, highest correlation coefficients were obtained for octanol–water partition coefficients and linear release rate constants. However, correlation coefficients were considerably higher for release without mastication than with mastication. Mastication/mouth movements are realistic conditions in the mouth. As physico-chemical characteristics poorly correlated with those data involving mastication, these characteristics

Table 6
Spearman correlation coefficients of linear release rate constants (k) and physico-chemical characteristics[a] of aroma compounds released from sunflower oil or water in a model mouth system, with and without mastication

Compound	Without mastication		With mastication	
	k_{water}	k_{oil}	k_{water}	k_{oil}
Molecular weight	0.930	−0.192	0.774	−0.167
Boiling point	0.857	−0.292	0.767	−0.116
Vapour pressure[b]	−0.201	−0.022	−0.196	0.464
Octanol-water partition coefficient (log P)[c]	0.802	−0.877	0.748	0.350
Gas-water partition coefficient[d]	0.920	−0.443	0.808	−0.120
Gas-oil partition coefficient[d]	−0.844	0.083	−0.786	0.317

[a] Molecular weights, boiling points at atmospheric pressure, saturated vapour pressure and octanol–water, gas–water and gas–oil partition coefficients.

[b] Vapour pressures calculated with Antoine equation (Reid, 1987), data presented in Fig. 1.

[c] Log P is based on literature data (Lide, 1997) presented in Fig. 1.

[d] Experimental data presented in Table 4.

alone are not suitable for prediction of aroma release under mouth conditions. In this dynamic process, mass transfer has to be taken into account.

4. Conclusions

The release of seven aroma compounds from an oil and water matrix, with and without mastication, for various time intervals was significantly influenced by the type of compound. Matrix composition and mastication affected the release, which effect varied with the compounds. Linear release rate constants of the aroma compounds differed considerably across the compounds, matrices and other conditions. The physico-chemical characteristics of the aroma compounds correlated only roughly with the linear release rate constants.

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