Food Chemistry 115 (2009) 843–851

Contents lists available at ScienceDirect

Food Chemistry

journal homepage: www.elsevier.com/locate/foodchem

Headspace volatiles contributing to flavour and consumer liking of wellness beverages

Terhi A. Pohjanheimo [a,*], Mari A. Sandell [a,b]

[a] Functional Food Forum, University of Turku, Kuuratie 4, 20014 Turku, Finland
[b] Department of Biochemistry and Food Chemistry, University of Turku, 20014 Turku, Finland

ARTICLE INFO

Article history:
Received 5 September 2008
Received in revised form 20 November 2008
Accepted 5 January 2009

Keywords:
Nutritionally fortified drink
SPME
OAV
Sensory quality
Health concern

ABSTRACT

The relationships between volatile composition, sensory profile and liking of four Finnish wellness beverages were determined. Wellness beverages are finely carbonated nutritionally fortified functional drinks and are a fast growing product category in many countries. The aroma compounds of wellness beverages were extracted by solid phase microextraction and analysed by a gas chromatography–mass spectrometer. The purpose of this experiment was to identify the sensory and chemical quality characters required for a positive hedonic response. The effect of consumers' health concerns on liking was also studied. This paper demonstrates that ethyl hexanoate, α-pinene, 3-hexenol, and hexyl acetate contribute to citrus-like and fresh odours and increase the liking of wellness beverages. On the other hand, 2-heptanone, which correlated with the calcium content, creates an off-flavour that is not pleasant for the consumer. Consumers who were more concerned about their health rated the wellness beverages as more pleasant.

1. Introduction

The increasing interest in healthy and nutritious food has multiplied the number of new health-promoting products on the market. Wellness beverages (also known as nutritionally fortified functional drinks and health beverages) are finely carbonated and non-alcoholic drinks. They might be enriched with vitamins, minerals and/or fibre and have been created for different kinds of everyday situations and for people who want to keep fit and feel good. These types of drinks were launched at the turn of the millennium. Euromonitor International reported that approximately $80 million beverages were sold in the fortified/functional carbonates category in 2005, and it has been estimated that the sales were valued at more than $200 million in 2007 and are forecasted to grow to more than $350 million in 2010 (Fuhrman, 2007). Young adults are the target group for traditional soft drinks, but a much wider audience is interested in the healthier alternatives, such as wellness beverages (Theodore, 2008).

Recent studies on health-promoting food products have shown that health-related information tends to increase the behavioural measure of acceptability as a food choice (Stein, Nagai, Nakagawa, & Beauchamp, 2003). Similarly McFarlane and Pliner (1997) found that nutritional information increased young adults' willingness to try novel foods. Urala and Lähteenmäki (2003) recently conducted a study of consumers' reasons for choosing functional foods in different product categories in Finland. In the study, a wellness beverage was compared to an artificially sweetened carbonated soft drink, an energy drink and a carbonated soft drink. Urala and Lähteenmäki (2003) found that from 70% to over 90% of consumers chose the wellness beverage over the other beverages and most often the consumers mentioned health as their reason for the choice of the wellness beverage.

However, even though health-related information may increase the interest in a product, various studies have shown that the information does not necessarily increase the sensory properties, e.g. liking of a product (Kähkönen, Tuorila, & Lawless, 1997; Shepherd, Sparks, Bellier, & Raats, 1991; Stein et al., 2003). Therefore, the product is unlikely to be accepted unless consumers really like the flavour. The sensory quality of food, which is strongly affected by its chemical composition, plays an important role in its liking.

This paper examines the effect of flavour and headspace volatile compounds on the liking of wellness beverages. The relationship between sensory quality and chemical composition can only be studied when the samples are handled identically in both analyses. Moreover, sample handling should not affect the compositional ratios of the compounds studied. Characterising headspace volatiles using a solvent-free solid phase microextraction (SPME) minimises sample handling (Arthur & Pawliszyn, 1990). However, volatiles that contribute to the odour perceived while consuming a product need to be present above their sensory detection threshold. As a result, the odour activity values (OAVs; a ratio of their concentrations in the beverages to their odour thresholds in water) were

* Corresponding author. Tel.: +358 40 70 45 223; fax: +358 2 333 6862.
E-mail addresses: terhi.pohjanheimo@utu.fi (T.A. Pohjanheimo), mari.sandell@utu.fi (M.A. Sandell).

0308-8146/$ - see front matter © 2009 Elsevier Ltd. All rights reserved.
doi:10.1016/j.foodchem.2009.01.012

calculated. The primary aim of this study was to correlate headspace volatiles to the sensory quality of the wellness beverages.

A large number of studies have related instrumental compositional data to sensory quality in different food products. Sometimes these results have also been linked to consumer data. However, most of the studies have related average hedonic ratings to analytical (instrumental and sensory descriptive) values. Such approaches do not take into account individual differences among consumers. Because consumer populations are very heterogeneous in their likes and dislikes, it is important to identify the likings of more homogenous consumer groups. Consumer demographics (e.g. age and gender) are often used to segment consumers. In this study the consumers were segmented based on their health concerns. In other words, the second aim of this study was to examine the critical sensory and chemical (volatiles composition, pH, soluble solids and titratable acidity) quality characteristics of the wellness beverages that are required for a positive hedonic response in different consumer groups.

2. Materials and methods

2.1. Wellness beverages

Four commercial wellness beverages (Table 1) were purchased from a local supermarket or received directly from the manufacturer. Chosen products were market leaders in the wellness beverage category in Finland in 2005.

2.2. Chemicals

Methyl isobutanoate, ethyl butanoate, ethyl 2-methylbutanoate, 2-methylpropyl acetate, 3-methylbutyl acetate, hexyl acetate, myrcene and terpinolene were purchased from Aldrich (Steinheim, Germany). Ethyl hexanoate, butyl acetate, ocimene, limonene and carvone were from Fluka (Buchs, Switzerland). Alpha-terpineol was obtained from Haarmann and Reimer (Teterboro, NJ). Stock Sim Dis Paraffin Solution of *n*-alkanes C5–C20 was from AccuStandard Inc. (New Haven, CT). All the chemical aroma compounds that were used as reference compounds were at least 99.5% pure.

2.3. Determination of volatile compounds

The headspace volatile compound analysis was carried out by gas chromatography–mass spectrometry (GC–MS) using the solid phase microextraction technique (SPME). The SPME fibre used for aroma extraction was 2 cm of 50/30 μm StableFlex divinylbenzene/carboxen/polymethylsiloxane (DVB/CAR/PDMS) (Supelco, Bellefonte, PA). This fibre has previously been used to analyse a wide range of beverages such as sea buckthorn juice (Tiitinen, Hakala, & Kallio, 2006) and different dry gins (Vichi, Riu-Aumatell, Mora-Pons, Buxaderas, & Lopez-Tamames, 2005).

Various sampling times were tested to optimise the sampling conditions. Even though the longer extraction time (30 min) improved the uptake of less volatile compounds, a shorter extraction time (5 min) was selected for sampling. This procedure was considered more equivalent to the procedure in hedonic testing and sensory profiling where the subjects evaluated the samples first by sniffing.

For sampling, a 10 mL sample was measured into a 100 mL glass Erlenmeyer bottle, which was then sealed with butyl Teflon septa and a cap with an adapter. Extraction was performed at room temperature (22 °C) under magnetic stirring (80 rpm, Cat M6, Staufen, Germany). Stirring was chosen based on the better absorption shown in the study by Rocha, Ramalheira, Barros, Delgadillo, and Coimbra (2001). After 15 min of sample conditioning, the fibre was exposed to the sample headspace for 5 min and then immediately desorbed in the gas chromatograph injector. Volatiles were analysed in duplicate from two or three separate beverage production batches.

The GC used was a Shimadzu GCMS-QP5000 (Kyoto, Japan) coupled with a mass spectrometer. Helium was used as the carrier gas at an average flow rate of 1.6 mL/min. The capillary column used was RH-5ms+ (30 m × 0.25 mm i.d. × 0.25 μm d_f, Lab Alliance TM, Chromatix Separation Sciences). Column temperature was held at 35 °C for 6 min and increased to 75 °C at a rate of 10 °C/min and then to 100 °C at a rate of 1 °C/min, and finally to 230 °C at a rate of 28 °C/min, held for 5 min. The temperature of the injector was 260 °C and the time of desorption of the fibre into the injection port was 5 min. The temperature of the detector was 270 °C. Electron impact mass spectra were recorded at a voltage of 70 eV ionization energy over the 40–350 *m/z* mass range.

Identification of the compounds was based on chromatographic and mass spectral information, reference compounds and the literature (e.g. Rychlik, Schieberle, & Grosch, 1998; Vichi et al., 2005). Identification was considered as unambiguous in the case of a match with the retention times and mass spectra of defined reference compounds. When identification was based on comparison of the mass spectrum with those of the Wiley 229 library (Shimadzu Spectral Library) and Kovats indices available in the literature only, we considered the identification to be tentative. Kovats indices were determined with a homologous series of n-alkanes C5–C20.

Quantification was carried out using two internal standards and a calibration curve for nine reference compounds. Compounds were first diluted by a small amount of ethanol and then water. The internal standard stock solution contained 200 μL/L methyl 2-methylpropanoate and 200 μL/L carvone. For sampling, beverage samples were spiked with the internal standard stock solution to a final concentration of 2 μL/L. Selected standards differed in their

Table 1
Details of the wellness beverage samples in the study (nutritional information g/100 mL).

Identity and code	Light pineapple 'LP'	Fruity fibre drink 'FF'	Energising cranberry drink 'EC'	Light fruit with cranberry flavour 'LF'
Manufacturer	(Oy Hartwall Ab, Finland)	(Oy Sinebrychoff Ab, Finland)	(Oy Hartwall Ab, Finland)	(Oy Sinebrychoff Ab, Finland)
Description	A low-calorie beverage	A beverage to promote bowel health	An energising beverage	A low-calorie beverage
Energy/100 mL	8 kcal/35 kJ	40 kcal/160 kJ	38 kcal/160 kJ	10 kcal/50 kJ
Protein	0 g	0 g	0 g	0.1 g
Carbohydrates	2 g	8.8 g	9 g	3 g
Of which sugar	2 g	8.6 g	9 g	2.2 g
Fat	0 g	0 g	0 g	0 g
Nutritional fibre	0 g	1.0 g	1 g	0.5 g
Sodium	<0.01 g	0 g	<0.01 g	0 g
Other	Magnesium 30 mg, vitamin C 30 mg	Calsium 50 mg, vitamin C 36 mg, vitamin E 2 mg, vitamin A 120 μg	Vitamin C 30 mg, ginseng-extract 15 mg, caffeine 13 mg	

functional group, and methyl 2-methylpropanoate eluted at the beginning and carvone at the end of the run. An external reference solution of seven representative compounds was prepared in 0.2, 0.5, 1 and 2 μL/L final concentrations and was analysed after being spiked with internal standard solution in duplicate under the same sampling and analysis conditions described above. Relative response factors (RRF) for representative compounds were calculated with respect to the internal standard methyl 2-methylpropanoate and used in quantification of volatile compounds in samples. RRF = Area ratio/Weight ratio, where Area ratio = *A*(representative compound)/*A*(methyl 2-methylpropanoate) and Weight ratio = *C*(representative compound)/*C*(methyl 2-methylpropanoate). The concentrations of volatiles were calculated as *C*(compound *x*) = Area ratio in sample *1/RRF* *C*(methyl 2-methylpropanoate). The RRF chosen for each identified compound in the sample was based on retention time and functionality.

2.4. Calculation of odour activity values

Odour activity values for volatiles were calculated by dividing the quantified concentration by the respective odour threshold in water. However, this method produces only indicative results of the aroma model of the products studied. Here the odour threshold values used were extracted from previous studies in water (Fritsch & Schieberle, 2005; Khiari, Suffet, & Barrett, 1995; Leffingwell et al., 2006; Rychlik et al., 1998; Schieberle & Hofmann, 1997; Stahl, 1973), while our sample matrix was a carbonated beverage. Although the effect of the matrix on the odour threshold of volatiles cannot be ignored, various aroma recombination models have been successfully prepared using the odour threshold values in water while the food matrix has been grapefruit juice or beer (Buettner & Schieberle, 2001; Fritsch & Schieberle, 2005). OAVs can be used only tentatively to assess the contribution of a single compound to the overall aroma, but these values still give an aroma profile closer to that sensed by a human from foods, than pure concentrations.

2.5. Determination of pH, soluble solids and titratable acidity

pH, soluble solids and titratable acidity were analysed in triplicate. pH was determined with a pH metre (Mettler Toledo, GmbH MP220, Schwerzenbach, Switzerland) and the soluble solids by a 0–32 °Brix refractometer (Atago, Tokyo, Japan). To determine the acidity the beverages were titrated with 0.1 M NaOH to the end point observed with a phenolphthalein indicator, and the total acidity was calculated as citric acid (AOAC 12.008).

2.6. Descriptive sensory analysis

A sensory profile of beverages was obtained using generic descriptive analysis with a panel of 30 assessors, of which 20 were women and 10 were men (age 20–70, average 31.5). The general guidelines for the selection, training and monitoring for assessors (ISO 8586-1) were used. The assessors were chosen on the basis of their willingness, availability and ability to recognise selected odours, basic tastes, and flavour differences in the samples. Each assessor participated in four 1-h training sessions where the panel developed a lexicon of 13 attributes through consensus (Table 2). All four samples were evaluated by their intensity of each attribute on a line scale of 0–10 (0 = none, 10 = very strong) in triplicate during three sessions. The sample presentation order was randomised between and within assessors. All samples were coded by random 3-digit numbers. Each sample (about 20 mL) was poured from the original bottles into 100 mL white plastic bottles (Tamro, Vantaa, Finland), sealed with a cap and stored at 8 °C in a fridge prior to the sensory evaluations. Activated-carbon-filtered tap water was served for cleansing the palates between samples. Compusense five software (version 4.1.2, Compusense, Guelph, Canada) was used for data collection. The sensory profiling was carried out in the sensory laboratory of the Functional Foods Forum, University of Turku, Finland, which meets the ISO 8589-1988 standard.

2.7. Hedonic test

A total of 194 consumers (age 18–76, mean 37.8, 41 males and 151 females) were recruited to participate in a hedonic test. Consumers evaluated the pleasantness of odour and taste in each sample and rated their liking score using a labelled affective magnitude (LAM) scale (Schutz & Cardello, 2001). The rating scale was a 100 mm vertical line, with the interior scale points consisting of the labels of the nine-point hedonic scale (dislike extremely, dislike very much, dislike moderately, dislike slightly, neither like nor dislike, like slightly, like moderately, like very much and like extremely). The extreme end anchors were labelled as the greatest imaginable liking/disliking. The samples were served in 100 mL white plastic bottles (Tamro, Vantaa, Finland) without product

Table 2
Sensory descriptors used for wellness beverages.

Attribute	Description	Reference compound	Intensity level
Odour			
Odour intensity	Strength of odour		
Tropical fruitiness	Fruity odour typical to tropical fruits (mango, passion, banana and pineapple)		
Citrus-like fruitiness	Fruity odour typical to citrus fruits (lemon, orange and lime)	Lemon[a]/orange[a] 3:2	8
Berry	Odour of sweet berries (blueberry, raspberry, strawberry)	Blueberry[a]/rasberry[a]/strawberry[a] 3:3:2	7
Artificial	Artificial essence-like odour		
Freshness	Fresh odour		
Flavour			
Sweetness	Taste caused by sugars and other sweeteners	2% Fructose solution	5
Sour	Taste caused by organic acids	0.15% Citric acid	8
Fruity	Fruity flavour of tropical fruits	Fruit nectar[b]	8
Sweet berries	Berry flavour of sweet berries (blueberry, raspberry, strawberry)	Blueberry–rasberry flavoured juice[c]	8
Sour berries	Flavour of sour berries (currants, lingon, cranberry)		
Mouth feel			
Bubbling	Strength of bubbling and fizzing mouth feel		
Astringency	Tingling, drying mouth feeling	0.2% $AlSO_4$	9

[a] Jean Lenoir Le Nez du vin, France.
[b] Marli Vital fruit nectar + 10 vitamins, Marli, Finland.
[c] Grandi, Valio Oy, Finland.

information and stored at 12 °C in a fridge. The samples were coded with 3-digit numbers and the presentation order was randomised between the subjects. The test was conducted at separate location in a shopping centre, with a maximum of four subjects at a time and minimising all disturbing factors.

2.8. Health Concern-scale

In order to study the effect of health attitudes on liking, consumers participating in the hedonic test completed the Concern-scale (developed by Kähkönen, Tuorila, and Rita (1996)) just after the tasting session. The Concern-scale contains 10 items related to concern about food and health. For instance, subjects evaluated their degree of concern for 'getting a lot of calories in food', 'gaining weight' or 'the risk of coronary heart disease'. The subjects were asked to rate their degree of concern for each statement using a nine-point Likert scale ranking from "not at all concerned" (1) to "extremely concerned" (9). The scale has been used previously (Bower, Saadat, & Whitten, 2003; Kähkönen et al., 1996, 1997; Kähkönen & Tuorila, 1999) and its reliability has been confirmed by high Cronbach's alphas (>0.8).

2.9. Statistical analysis

Differences among samples were analysed by a one-way analysis of variance (ANOVA). Tukey's test and a Tamhane test were used for a multiple comparison of volatile composition, sensory attributes and liking at $p < 0.05$. The Concern-scale was constructed by computing the mean of the items. Consumers were divided into three groups depending on their scale values, using the 33rd and 66th percentile points as cut-off points. These groups were designated 'low', 'moderate' and 'high', depending on which third of the subjects they represented on the scale. SPSS 14.0 (Inc., Chicago, IL) was used for analysis.

Partial least square regression (PLSR) was performed using the statistical package Unscrambler version 9.7 (Camo, Trondheim, Norway). PLSR was used to understand the correlation between the odour activity values (OAVs) of the volatile compounds and the sensory descriptors, and to study the relationship between sensory and instrumental quality and consumers' liking of beverage samples. The data were standardised and full cross validation was used as the validation criterion.

Table 3
Quantitative data of volatile compounds identified in the headspace of the wellness beverages – light pineapple (LP), fruity fibre (FF), energising cranberry (EC) and light fruit (LF).

Number	Compound	ID[a]	KI[b]	RRF[c]	Concentration (mg/L) ± standard deviation[d]			
					(LP)	(FF)	(EC)	(LF)
1	Ethyl acetate	T	625	E	1.13 ± 0.60	1.75 ± 0.36	1.66 ± 0.39	1.34 ± 0.67
2	Ethyl propanoate	T	701	F	nf	nf	0.20 ± 0.05	nf
3	2-Methylpropyl acetate	S	767	F	nf	0.61 ± 0.08	0.80 ± 0.21	nf
4	Ethyl butanoate	S	799	G	1.33 ± 0.14	0.95 ± 0.07	1.00 ± 0.43	0.21 ± 0.06
5	Butyl acetate	S	819	H	<0.03	0.17 ± 0.10	nf	nf
6	Ethyl 2-methylbutanoate	S	858	I	0.45 ± 0.06	nf	1.00 ± 0.11	nf
7	Ethyl 3-methylbutanoate	S	862	I	nf	nf	nf	0.03 ± 0.01
8	3-Hexenol	T	868	I	<0.03	nf	nf	nf
9	1-Hexanol	S	877	I	<0.03	<0.03	nf	nf
10	3-Methylbutyl acetate	S	884	I	1.10 ± 0.16	1.09 ± 0.08	nf	nf
11	2-Heptanone	T	895	I	nf	0.03 ± 0.02	nf	nf
12	α-Pinene	T	928	I	0.06 ± 0.06	<0.03	nf	nf
13	2-Methylpropyl butanoate	T	953	I	0.18 ± 0.03	0.09 ± 0.01	nf	nf
14	Benzaldehyde	S	956	I	<0.03	<0.03	nf	nf
15	Myrcene	S	990	J	0.36 ± 0.18	0.14 ± 0.01	<0.03	0.50 ± 0.08
16	Butyl butanoate	S	995	J	nf	<0.03	<0.03	nf
17	Ethyl hexanoate	S	999	J	1.65 ± 0.23	0.43 ± 0.33	0.62 ± 0.12	<0.03
18	Unknown: 41 (100), 43(45), 55 (20), 67 (18), 69 (22), 77 (25), 79 (18), 91 (30), 93 (50), 105 (4)		1000	J	nf	nf	nf	0.03 ± 0.01
19	(Z)-3-hexenyl acetate	T	1005	J	0.27 ± 0.05	0.18 ± 0.04	0.27 ± 0.07	nf
20	α-Terpinene	T	1011	J	nf	nf	nf	0.09 ± 0.02
21	Hexyl acetate	S	1012	K	0.79 ± 0.18	nf	<0.03	nf
22	Limonene	S	1029	L	7.06 ± 1.76	4.97 ± 0.94	0.14 ± 0.07	10.95 ± 2.03
23	Unknown: 41 (75), 43 (100), 67 (85), 68 (62), 79 (60), 93 (95), 105 (20), 107 (22), 119 (28), 121 (23)	T	1033	L	<0.03	<0.03	nf	<0.03
24	Trans-ocimene	T	1042	L	<0.03	<0.03	nf	<0.03
25	Unknown: 41 (40), 43 (100), 55 (42), 70 (59), 71 (60), 89 (13), 101 (1), 115 (3)	T	1050	L	nf	0.13 ± 0.03	nf	nf
26	γ-Terpinene	T	1052	L	0.07 ± 0.03	nf	nf	0.03 ± 0.01
27	Terpinolene	T	1078	L	0.07 ± 0.03	0.04 ± 0.01		0.12 ± 0.03
28	Propyl hexanoate	T	1090	L	nf	0.12 ± 0.02	nf	nf
29	Linalool	S	1095	L	<0.03	<0.03	nf	nf
30	Nonanal	T	1104	L	<0.03	nf	<0.03	nf
31	Butyl hexanoate	T	1144	L	0.10 ± 0.02	nf	nf	nf
32	(Z)-3-hexenyl-butanoate	T	1179	L	0.11 ± 0.03	0.23 ± 0.03	nf	nf
33	Unknown: 41(50), 43 (70), 59 (100), 67 (50), 68 (45), 81 (38), 93 (70), 107 (10), 121 (40), 136 (30)	T	1180	L	nf	nf	nf	<0.03
34	Decanal	S	1209	L	<0.03	<0.03	<0.03	nf
35	(Z)-3-hexenyl hexanoate	T	1354	M	0.42 ± 0.17	nf	nf	nf
36	Hexyl hexanoate	T	1355	M	0.90 ± 0.31	nf	nf	nf

nf: Not found.
[a] Identification method: S: mass spectra and retention time consistent with that of a standard and T: tentatively identified by mass spectra and Kovats indices.
[b] Kovats indices were calculated on a RH-5ms+ column using *n*-alkanes C5–C20.
[c] Relative response factor employed for quantification: E: RRF of methyl 2-methylpropanoate (RRF = 1); F: RRF of 2-methylpropyl acetate (2.67); G: RRF of ethyl butanoate (1.99); H: RRF of butyl acetate (2.38); I: RRF of ethyl 2-methylbutanoate (3.50); J: RRF of ethyl hexanoate (5.36); K: RRF of hexyl acetate (6.06); L: RRF of limonene (7.66); and M: RRF of carvone (0.10).
[d] Mean concentration of 4–6 analysis ± standard deviation.

3. Results and discussion

3.1. Volatile compounds

A satisfactory linearity of responses in the total ion chromatograms was obtained for external reference compounds; the correlation coefficients calculated for each volatile with four calibration points varied from 0.985 to 0.998. Repeatability of the analyses was found to be acceptable by examining the peak areas of internal standard compounds in all runs. Carvone was also used to confirm the quantification results by calculating the concentration of carvone as 2 μL/L in all samples. Additionally, the quantification results were verified by doubling the calculated concentration of ethyl butanoate or ethyl hexanoate in the samples and detecting the doubling in the peak area (data not shown). A total of 36 volatile compounds were identified. The results are described in Table 3, together with the identification methods employed. The majority of compounds were esters (18) followed by monoterpenes (6), aldehydes (3) alcohols (2) and ketones (1). Table 3 also presents the mean concentrations of volatile compounds found in each sample, expressed in milligrams per litre and the RRF used for quantification. Four beverage samples differed in their volatile composition. Ethyl acetate, ethyl butanoate, ethyl 2-methylbutanoate, 3-methylbutyl acetate and ethyl hexanoate were the esters found at the highest concentrations. The concentration of ethyl butanoate was high in the pineapple (LP) and cranberry (EC) samples (>1 mg/L) compared with the light fruit (LF) sample, ethyl 2-methylbutanoate was highest in the EC beverage, 3-methylbutyl acetate was highest in the LP and fruity fibre (FF) samples, and ethyl hexanoate in the LP sample. Limonene was the monoterpene found at the highest concentration in light fruit (LF), pineapple (LP) and fruity fibre (FF) beverages (concentration between 5.0 and 11.0 mg/L), while in EC the concentration was low (0.1 mg/L).

The odour activity values (OAVs) were calculated on the basis of the odour thresholds in water. Calculation of the odour activity values (Table 4) revealed four compounds as the most odour-active, namely ethyl butanoate, ethyl 2-methylbutanoate, ethyl hexanoate and limonene. The odour quality of these compounds is described as an apple, fruit and citrus type (Acree & Arn, 2006; Rychlik et al., 1998).

3.2. Sensory profile

The sensory profiles of the wellness beverages determined by the sensory panel are shown in Fig. 1. Statistical analysis revealed significant differences ($p < 0.05$) between the samples in 11 out of 13 attributes evaluated. No differences in artificial odour and sweet taste were observed between samples. The strongest differences were in berry-like odour ($F = 214.5$, $p < 0.001$), sour berry-like flavour ($F = 213.2$, $p < 0.001$) and fruity flavour ($F = 138.6$, $p < 0.001$). The light fruit (LF) sample was generally described as the strongest in berry-like odour and flavour, whereas the fruity fibre (FF) sample was the most intense in overall odour intensity, tropical fruitiness and fruity flavour.

The ingredients of each wellness beverage are shown in Table 1. When manufacturers formulate nutritionally fortified drinks, they may face significant flavour challenges due to the addition of vitamins, minerals or other ingredients (Eckert & Riker, 2007). For example, in those beverages studied here, the energising cranberry (EC) beverage may have been challenging to produce because it contains caffeine, which elicits bitterness that is not necessarily a desired characteristic for a beverage. Keast (2008) studied different strategies for suppressing the bitterness of caffeine and reported that the sweetness of sucrose can decrease the observed bitterness. Adding caffeine to the wellness beverages may thus require the addition of sugars, as was the case in the EC beverage. However, this defines the caloric content of the beverage. Other methods for suppressing bitterness should be studied if a manufacturer wants to produce a low-calorie product containing caffeine. Adding calcium or vitamins may also create different off-flavours. The taste of calcium has been described as moderately bitter, smooth and flat (Tordoff, 2001). Fruity fibre (FF) was the only beverage containing calcium and its sensory profile differed from the others, being significantly ($p < 0.05$) less fresh in flavour.

Table 4
Odour thresholds, odour activity values (OAVs) and odour quality of volatile compounds in wellness beverages.

	Compound	Odour threshold in water[a] (μg/L)	OAV[b] in LP	OAV[b] in FF	OAV[b] in EC	OAV[b] in LF	Odour quality[c]
1	Ethyl acetate	5	226	350	332	268	Pineapple
2	Ethyl propanoate	10			20		Fruit
3	2-Methylpropyl acetate	66		9	12		Fruit, apple, banana
4	Ethyl butanoate	1	1330	950	1000	220	Apple
5	Butyl acetate	66	<1	3			Pear
6	Ethyl 2-methylbutanoate	0.15	3000		6666		Apple
7	Ethyl 3-methylbutanoate	0.2				150	Fruit
8	3-Hexenol	70	<1				Grass
9	1-Hexanol	2500	<1	<1			Flower, green
10	3-Methylbutyl acetate	2	550	545			Banana, fruit
11	2-Heptanone	140		1			Soap
12	α-Pinene	6	10	3			Pine, terpeny
14	Benzaldehyde	350–3500	<1	<1			Almond, burnt sugar
15	Myrcene	13–15	24–28	9–11	<1	35–40	Balsamic, must, spice
16	Butyl butanoate	100		<1	<1		
17	Ethyl hexanoate	1	1650	430	620	20	Apple-peel, fruit
19	(Z)-3-hexenyl acetate	2	135	90	135		Green, banana, sweet, grass
21	Hexyl acetate	2	395		10		Fruit, herb
22	Limonene	10	706	497	14	1095	Lemon, orange
27	Terpinolene	200	<1	<1		<1	
29	Linalool	0.14	71	71			Flowery, citrus
30	Nonanal	1	10		10		Fat, citrus, green
31	Butyl hexanoate	700	<1				
34	Decanal	1	20	10			Orange peel, soap

[a] Odor thresholds (Fritsch & Schieberle, 2005; Khiari et al., 1995; Leffingwell & Associate, 2006; Schieberle & Hofmann, 1997; Stahl 1973).
[b] Odour activity values were calculated by dividing the quantified concentration (mg/L) of the odourants by their odor detection threshold (μg/L) in water.
[c] Odour characteristics (Acree & Arn, 2006; Rychlik et al., 1998).

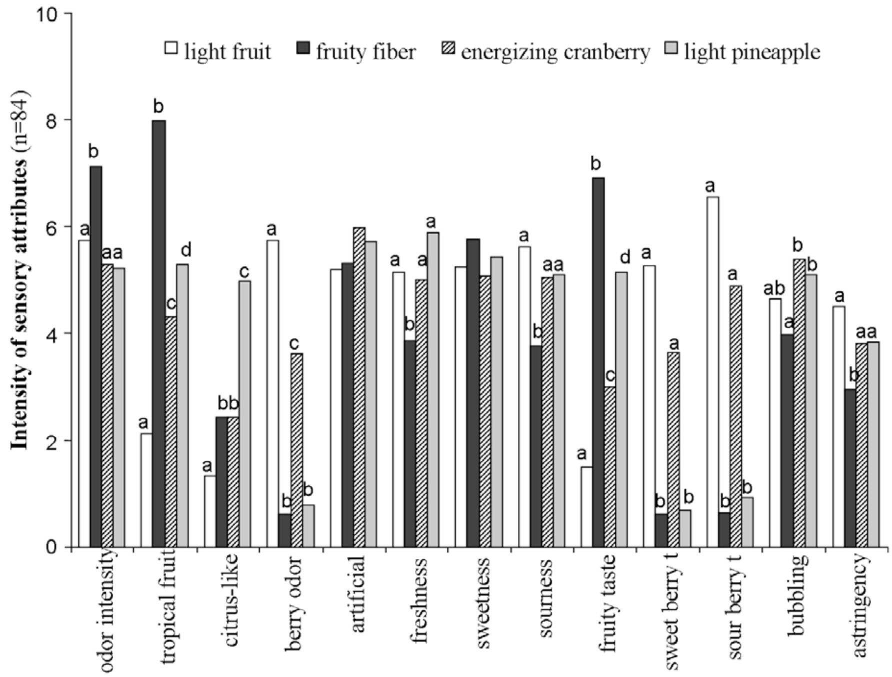

Fig. 1. The results of the sensory descriptive analysis. Letters a–d indicate that the sensory characteristics are significantly different between the samples ($p < 0.05$). No letters were added if there was no difference.

3.3. Correlation between sensory profile and volatile compounds

The PLSR method was used to relate the sensory data and OAVs of the volatiles (Fig. 2). Sixty-five percent of the volatile variables explained 91% of the sensory properties with the first two principal components. The first PC described the variability of sweetness and sourness. Sour taste, astringent mouth feeling and berry-like flavour are located on the opposite side to sweetness, fruity flavour and tropical fruitiness. It can be seen that sensory-related sweetness is mostly explained by butyl acetate ($r = 0.96$, $p < 0.05$), which has a pear-like odour Acree and Arn, 2006). Based on the results of the loading plot and high correlation coefficients we suggest that 3-methylbutyl acetate, butyl acetate and linalool are responsible for the tropical odour and fruity flavour. Sample LP, which had

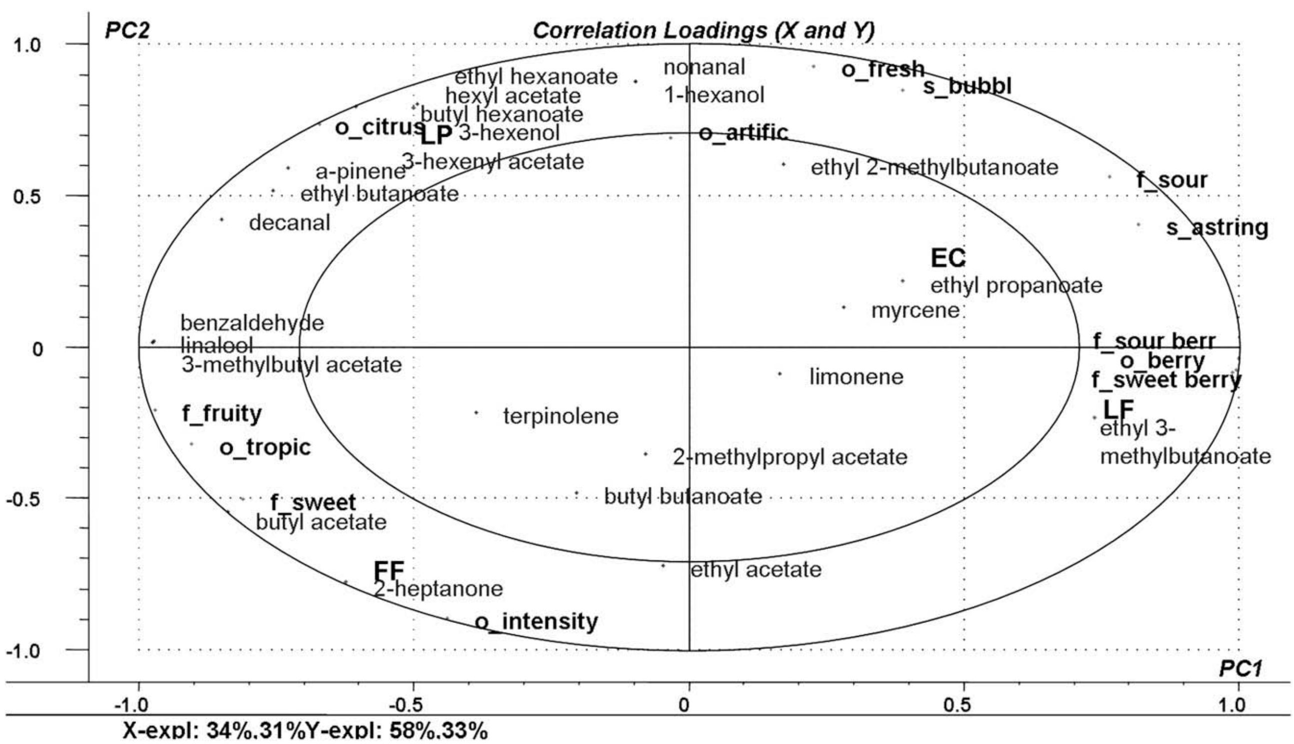

Fig. 2. Correlation loading plot from a partial least squares regression (PLSR) model based on OAVs of volatile compounds as predictors and descriptive sensory attributes as response variables. The inner and outer ellipses represent 50% and 100% of explained variance, respectively.

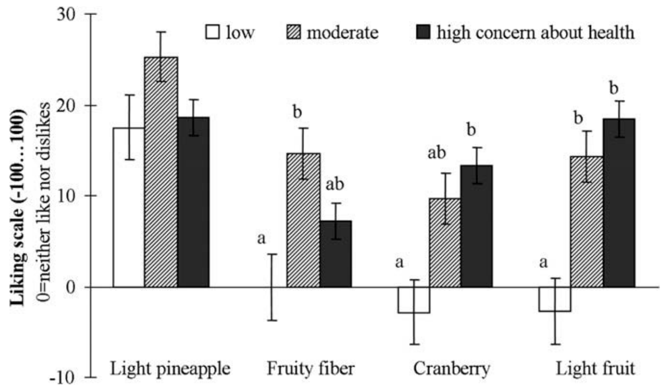

Fig. 3. Consumer evaluations of wellness beverages. The overall pleasantness ratings by the concern groups (low, moderate or high concern about health). Letters a–b indicate that the consumer segments differ significantly ($p < 0.05$) in liking. No letters were added if there was no difference. The LAM liking scale varies between –100…100 ± SE, where 0 means "neither like nor dislike".

the highest score of sensory-related citrus odour, was characterised by α-pinene, ethyl hexanoate, hexyl acetate, 3-hexenol, 3-hexenyl acetate and butyl hexanoate (pine, apple-peel, grass and fruit-like odours). Compounds 1-hexanol and nonanal (green and citrus-like odours) had a strong positive correlation with sensory-related freshness, but together with ethyl-2-methylbutanoate (apple-like odour) the volatiles also produced an artificial essence-like odour.

The second PC described a strong negative correlation between the sensory characteristics of fresh odour and odour intensity together with 2-heptanone. 2-heptanone was detected only in the FF beverage. Acree and Arn (2006) and Rychlik et al. (1998) reported that 2-heptanone contributed to a soapy smell. Interestingly, Tordoff (2001) reported that calcium causes a soap-like odour. This was consistent with our study, as fruity fibre was the only beverage that was fortified with calcium and also characterised by 2-heptanone. It is possible that calcium and 2-heptanone interact with each other in the FF beverage. Strong positive correlation between calcium and 2-heptanone concentrations has previously been described in cheeses (e.g. Lawlor, Delahunty, Wilkinson, & Sheehan, 2002) and in sausages (Flores, Nieto, Ferrer, & Flores, 2005).

3.4. Liking of wellness beverages

A significant difference in liking was detected between wellness beverages when hedonic scores were averaged over all 194 consumers. The most liked beverage was the light pineapple (LP) which was rated significantly higher in the liking scale than the other samples ($p < 0.001$). Light pineapple was rated between the anchors 'like slightly' and 'like moderately', while other beverages were rated between 'neither like nor dislike' and 'like slightly' on the LAM scale.

A high Cronbach's alpha (0.85) was calculated for the Concern-scale which indicates good reliability. Individual means of concern varied from 1.9 to 8.8, and subjects were divided into three subgroups based on how concerned they were. The 'low' group ($n = 57$) was not worried about health (mean score 3.9), while the 'high' group ($n = 63$) was relatively worried (mean score 7.6) and the 'moderate' group ($n = 65$) was in between (mean score 5.7). The mean Concern score correlated significantly with age ($r = 0.45$, $p < 0.001$). The mean age was 46 years in the 'high' concern group, 34 years in the 'moderate' group while unconcerned consumers were on average 32 years old. This means that older subjects were more concerned about health and food, similar to results obtained previously (Bower et al., 2003).

These three groups differed significantly ($p < 0.05$) in how much they liked the wellness beverages (Fig. 3). All of the sub-groups considered light pineapple to be the most pleasant beverage. Subjects who were more concerned about their health, i.e. 'moderate' and 'high' sub-groups, gave higher scores for all other three

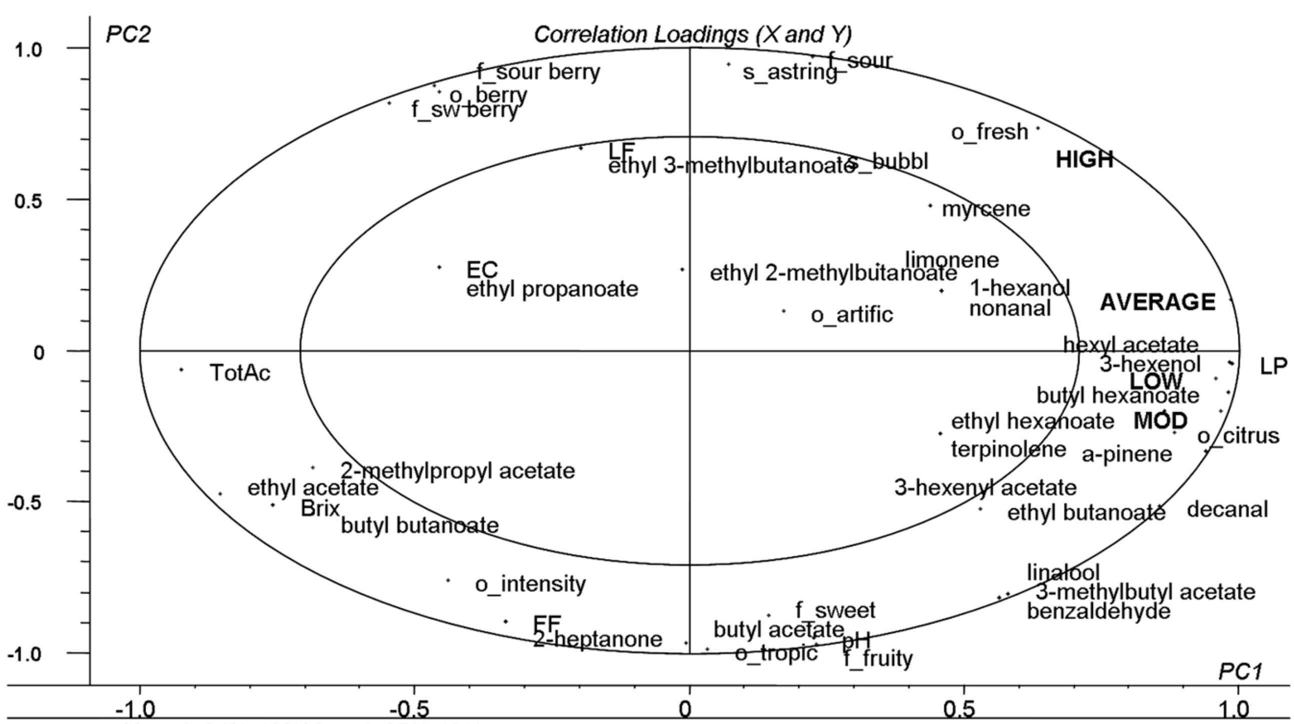

Fig. 4. Correlation loading plot from a PLSR model based on liking of wellness beverages (y = consumer average, consumer sub-groups 'low', 'moderate' and 'high' concern) and product-related characteristics (x = sensory attributes, OAVs of volatile compounds, pH, Brix and titratable acidity).

wellness beverages than the ‘low’ sub-group. Consumers knew that they were evaluating wellness beverages and this may have influenced the concerned consumers more. The concerned consumers were interested in influencing their own health by consuming healthy products. This is consistent with a previous sensory experiment where information on reduced-fat content increased the pleasantness ratings of different food products only in health-concerned consumers (Kähkönen & Tuorila, 1999).

PLSR was performed to examine which sensory characteristics as well as volatile compounds, pH, Brix and titratable acidity could explain the liking of the wellness beverages in the different consumer segments (Fig. 4). Seventy-four percent of the product-related characteristics (sensory and chemical quality) explained a total of 97% of the liking data variance with the first two PLSR components. The ‘moderate’ and ‘low’ sub-groups were located near each other. The liking scores of the ‘moderate’ and ‘low’ concern groups correlated with citrus-like odour and volatiles characterised by fruit, apple-peel, grass and pine-like odours (3-hexenol, α-pinene, ethyl hexanoate, hexyl acetate, butyl hexanoate and decanal). Based on a negative correlation, these unconcerned subjects considered high acidity (measured as titratable acidity) as a non-pleasant characteristic. The second PC described the difference between concerned and unconcerned subjects. Unlike in less concerned consumers, important properties for the ‘high’ concern subjects were fresh odour and volatiles characterised by lemon, green, balsamic and fruit-like odours (limonene, 1-hexanol, myrcene and ethyl 3-methylbutanoate), and to some extent sour taste, astringent and bubbling mouth feeling. A sensory-related sweet taste, fruity flavour, high Brix and pH, and volatiles characterised by pineapple, banana and pear (ethyl acetate, 2-methylpropyl acetate and butyl acetate) were negative drivers of liking for the health-concerned consumers. In other words, the concerned and older subjects considered sourness and astringency as more pleasant characteristics than sweetness and fruity flavour in wellness beverages than the unconcerned subjects. Luckow and Delahunty (2004) found a similar result in their studies with probiotic and conventional non-dairy juice drinks. They found that older consumers (over 40) rated the more sour and perfumey probiotic beverage as more pleasant than younger consumers, and later guessed that their most preferred juice was the healthiest sample. Luckow and Delahunty (2004) presumed that the reason for the difference between the age groups might be the decreased chemical sensitivity that occurs with age, or because older consumers might be more accepting of uncharacteristic sensory attributes in a healthy product. However, Tuorila and Cardello (2002) found that increasing the intensity of an off-flavour in juice (increasing the concentration of KCl increased sourness and bitterness, and decreased sweetness) decreased the ratings of liking although information about a health benefit enhanced the liking of a product. No health benefits were claimed in our study but the consumers were aware that the products belonged to the category of wellness beverages. However, this might have been sufficient for the health-concerned subjects to be more positive towards the samples.

4. Conclusion

This study examined four Finnish wellness beverages that had a different composition and differed from each other in terms of their flavour and headspace volatile compounds. Healthy beverages fortified with a variety of vitamins, minerals and/or fibres are becoming increasingly important as beverage manufacturers seek to diversify their product range to meet consumer demands. We demonstrated that it is possible to study the volatile compounds corresponding to single sensory characteristics by calculating odour activity values and minimising handling of samples. odour and flavour attributes of these beverages determined by a sensory panel were correlated with subsets of volatile compounds. In general, consumers liked wellness beverages characterised by a citrus-like odour and volatiles characterised by 3-hexenol, nonanal, hexyl acetate and ethyl hexanoate (grass, citrus, fruit, apple-peel type of odours). We found that a wellness beverage containing calcium correlated strongly with 2-heptanone (a soapy odour). To avoid unwanted off-flavours, manufacturers need to pay extra attention to the sensory quality of beverages fortified with vitamins and/or minerals. In this study, the importance of sensory and chemical quality characteristics was perceived differently by health-concerned and unconcerned subjects. For the unconcerned subjects, the sensory-related citrus odour and volatiles characterised by hexyl acetate, butyl hexanoate, α-pinene, decanal and 3-hexenyl acetate (fruit, pine, orange peel, banana) were the positive drivers of liking, while the concerned subjects gave higher scores to all of the beverages and considered sourness and astringency as positive characteristics.

Acknowledgements

The authors would like to acknowledge TEKES (the Finnish Funding Agency for Technology and Innovation) and ABS (The Finnish Graduate School on Applied Bioscience: Bioengineering, Food and Nutrition, Environment) which partly funded this research. Professor Heikki Kallio is thanked for helpful scientific discussions, Ms. Anne Rantala for her assistance in the sensory analysis, Ms. Merja Laakso for her technical assistance and M.Sc. Rami Paasovaara for his assistance in the consumer test.

References

Acree, T., & Arn, H. (2006). *Flavornet and human odor space*. Retrieved 15.12.06. <http://flavornet.org/flavornet.html>.

Arthur, C. L., & Pawliszyn, J. (1990). Solid phase microextraction with thermal desorption using fused silica optical fibers. *Analytical Chemistry, 62*(19), 2145–2148.

Bower, J. A., Saadat, M. A., & Whitten, C. (2003). Effect of liking, information and consumer characteristics on purchase intention and willingness to pay more for a fat spread with a proven health benefit. *Food Quality and Preference, 14*(1), 65–74.

Buettner, A., & Schieberle, P. (2001). Evaluation of key aroma compounds in hand-squeezed grapefruit juice (*Citrus paradisi* Macfayden) by quantitation and flavor reconstitution experiments. *Journal of Agricultural and Food Chemistry, 49*(3), 1358–1363.

Eckert, M., & Riker, P. (2007). Overcoming challenges in functional beverages. *Food Technology, 61*, 20–26.

Flores, M., Nieto, P., Ferrer, J. M., & Flores, J. (2005). Effect of calcium chloride on the volatile pattern and sensory acceptance of dry-fermented sausages. *European Food Research and Technology, 221*, 624–630.

Fritsch, H. T., & Schieberle, P. (2005). Identification based on quantitative measurements and aroma recombination of the character impact odorants in a Bavarian Pilsner-type beer. *Journal of Agricultural and Food Chemistry, 53*(19), 7544–7551.

Fuhrman, E. (2007). *Health and wellness happenings*. Beverage Industry, February Issue. www.bevindustry.com.

Keast, R. S. J. (2008). Modification of the bitterness of caffeine. *Food Quality and Preference, 19*(5), 465–472.

Khiari, D., Suffet, I., & Barrett, S. (1995). Extraction and identification of chemicals causing grassy odors in flavor profile analysis (FPA) reference standards. *Water Science and Technology, 31*(11), 93–98.

Kähkönen, P., & Tuorila, H. (1999). Consumer responses to reduced and regular fat content in different products: Effects of gender, involvement and health concern. *Food Quality and Preference, 10*(2), 83–91.

Kähkönen, P., Tuorila, H., & Lawless, H. (1997). Lack of effect of taste and nutrition claims on sensory and hedonic responses to a fat-free yogurt. *Food Quality and Preference, 8*(2), 125–130.

Kähkönen, P., Tuorila, H., & Rita, H. (1996). How information enhances acceptability of a low-fat spread. *Food Quality and Preference, 7*(2), 87–94.

Lawlor, J. B., Delahunty, C. M., Wilkinson, M. G., & Sheehan, J. (2002). Relationships between the gross, non-volatile and volatile composition and the sensory attributes of eight hard-type cheeses. *International Dairy Journal, 12*(6), 493–509.

Leffingwell et al. (2006). Retrieved 8.12.06. <http://leffingwell.com/odorthre.htm>.

Luckow, T., & Delahunty, C. (2004). Which juice is ‘healthier’? A consumer study of probiotic non-dairy juice drinks. *Food Quality and Preference, 15*(7–8), 751–759.

McFarlane, T., & Pliner, P. (1997). Increasing willingness to taste novel foods: Effects of nutrition and taste information. *Appetite, 28*(3), 227–238.

Rocha, S., Ramalheira, V., Barros, A., Delgadillo, I., & Coimbra, M. A. (2001). Headspace solid phase microextraction (SPME) analysis of flavor compounds in wines. Effect of the matrix volatile composition in the relative response factors in a wine model. *Journal of Agricultural and Food Chemistry, 49*(11), 5142–5151.

Rychlik, M., Schieberle, P., & Grosch, W. (1998). *Compilation of odor thresholds, odor qualities and retention indices of key food odorants*. Deutsche Forschunganstalt fur Lebensmittelchemie and Institut fur Lebensmittelchemie der Technischen Universität Munchen, D-85748 Garching, Germany.

Schieberle, P., & Hofmann, T. (1997). Evaluation of the character impact odorants in fresh strawberry juice by quantitative measurements and sensory studies on model mixtures. *Journal of Agricultural and Food Chemistry, 45*(1), 227–232.

Schutz, H. G., & Cardello, A. V. (2001). Labeled affective magnitude (LAM) scale for assessing food liking/disliking. *Journal of Sensory Studies, 16*, 117–159.

Shepherd, R., Sparks, P., Bellier, S., & Raats, M. M. (1991). The effects of information on sensory ratings and preferences: the importance of attitudes. *Food Quality and Preference, 3*(3), 147–155.

Stahl, W. H. (1973). *Compilation of odor and taste threshold values data*. Philadelphia, PA: American Society for Testing and Materials.

Stein, L. J., Nagai, H., Nakagawa, M., & Beauchamp, G. K. (2003). Effects of repeated exposure and health-related information on hedonic evaluation and acceptance of a bitter beverage. *Appetite*, 40 119–129.

Theodore, S. (2008). *Beverage R&D: Banking on boomers*. Beverage Industry. Posted 07.15.08. www.bevindustry.com.

Tiitinen, K., Hakala, M., & Kallio, H. (2006). Headspace volatiles from frozen berries of sea buckthorn (*Hippophae rhamnoides* L.) varieties. *European Food Research and Technology, 223*(4), 455–460.

Tordoff, M. G. (2001). Calcium: taste, intake, and appetite. *Physiological Reviews, 81*(4), 1567–1597.

Tuorila, H., & Cardello, A. V. (2002). Consumer responses to an off-flavor in juice in the presence of specific health claims. *Food Quality and Preference, 13*(7–8), 561–569.

Urala, N., & Lähteenmäki, L. (2003). Reasons behind consumers' functional food choices. *Nutrition & Food Science, 4*, 144–158.

Vichi, S., Riu-Aumatell, M., Mora-Pons, M., Buxaderas, S., & Lopez-Tamames, E. (2005). Characterization of volatiles in different dry gins. *Journal of Agricultural and Food Chemistry, 53*(26), 10154–10160.