Available online at www.sciencedirect.com
SCIENCE DIRECT®
Food Chemistry 98 (2006) 343–350
Food Chemistry
www.elsevier.com/locate/foodchem

Characterisation of the volatile profiles of infant formulas by proton transfer reaction-mass spectrometry and gas chromatography–mass spectrometry

Saskia M. van Ruth *, Vincent Floris, Stéphane Fayoux

Department of Food and Nutritional Sciences, University College Cork, Western Road, Cork, Ireland

Received 31 January 2005; accepted 10 June 2005

Abstract

The volatile profiles of 13 infant formulas were evaluated by proton transfer reaction-mass spectrometry (PTR-MS) and gas chromatography–mass spectrometry (GC–MS). The infant formulas varied in brand (Aptamil, Cow & Gate, SMA), type (for different infant target groups) and physical form (powder/liquid). Fingerprint mass spectra were obtained from the headspace of the samples using PTR-MS. GC–MS was used to identify the volatile compounds. Brand, type and physical form of the infant formulas had a significant effect on the volatile profiles measured by PTR-MS. Forty-two masses were significantly affected by the brand, 14 by the type of formula, and 40 by the physical form. Eleven masses were among the most abundant across all samples (mass m/z 43, 45, 49, 55, 59, 60, 63, 69, 73, 83, and 87). Gas chromatography–mass spectrometry revealed the identity of 28 of the volatile compounds of the infant formulas. Most of the masses detected in PTR-MS were related to compounds identified by GC–MS.

Keywords: Aroma compounds; GC-MS; Infant; PTR-MS; Volatile compounds

1. Introduction

Early flavour experiences influence later food and flavour preferences in humans. Menella, Jagnow, and Beauchamp (2001) showed that prenatal and early postnatal exposure to a flavour enhanced the infants' enjoyment of that flavour in solid foods during weaning. Some studies reported that flavour experiences with mothers' milk, resulting from flavours transmitted from the mothers' diet, modify and serve to establish preferences (Menella & Beauchamp, 1999). Flavours, either consumed by the mother and transmitted to her milk or added to formula were shown to be detected by the infant and served to modulate feeding (Menella & Beauchamp, 1996). For those infants who are not breastfed, infant formula serves as the sole source of nutrition during infancy, and particularly during the first four to six months of life. With regard to infant formula specifically, it has been shown that flavour preferences of 4- and 5-year old children differed as a function of the class of formula they were fed during their infancy (Menella & Beauchamp, 2002). For instance, children fed soy formulas preferred bitter-flavoured apple juice instead of plain or sour-flavoured apple juice. Children fed protein hydrolysate formulas were more likely to prefer sour-flavoured juices. These data showed that flavour experiences influence subsequent flavour preferences even several years following the early experience.

It is generally thought that commercially available infant formulas differ considerably in flavour. However, very few studies on the characterisation of the flavour of infant formulas have been reported. Fenaille, Visani, Fumeaux, Milo, and Guy (2003) reported a study

* Corresponding author. Present address: RIKILT - Institute of Food Safety, PO Box 230, 6700 AE Wageningen, The Netherlands. Tel.: +31 317 475 414; fax: +31 317 417 717.
E-mail address: saskia.vanruth@wur.nl (S.M. van Ruth).

0308-8146/$ - see front matter © 2005 Elsevier Ltd. All rights reserved.
doi:10.1016/j.foodchem.2005.06.012

involving the comparison of two analytical techniques to assess oxidation in infant formulas.

Flavour volatiles in infant formulas are likely to be formed mainly in Maillard reactions and lipid oxidation reactions. The high lactose and lysine contents of the infant formula powders, the relatively high temperatures applied during the manufacturing process, the packaging conditions and storage for long periods of time make the infant formulas susceptible to Maillard reactions (Ferrer, Alegría, Farré, Abellán, & Romero, 2005; Albalá-Hurtado, Veaciana-Nogués, Mariné-Font, & Vidal-Carou, 1998). Lipid oxidation is well recognised as a major cause of quality deterioration during processing or storage of lipid-rich foods like dried milk powders. During peroxidation of unsaturated fatty acids, hydroperoxides are formed and these primary products decompose to form a complex mixture of secondary lipid oxidation products (alkanes, alkenes, aldehydes, ketones). Powder infant formulas are rich in polyunsaturated fatty acids such as $n-6$ arachidonic acid (C20:4, $n-6$) and $n-3$ docosahexaenoic acid (C22:6, $n-3$). These fatty acids are very susceptible to oxidation. In addition, linoleic acid (C18:2, $n-6$) is an important compound with regard to lipid oxidation products because of its relatively high concentration in infant formulas. The development of a number of aldehydes has been examined in infant formulas in order to follow lipid oxidation. Without daylight, extended storage resulted in high concentrations of propanal, pentanal, hexanal, heptanal and nonanal (Romeu-Nadal, Castellote, & López-Sabater, 2004; Ulberth & Roubicek, 1995). Pentanal and hexanal are the specific volatile oxidation products of $n-6$ polyunsaturated fatty acids and propanal is a product of $n-3$ polyunsaturated fatty acids (Romeu-Nadal et al., 2004) confirming the importance of lipid oxidation for the volatile composition of infant formulas. Apart from these aldehydes and some furfurals resulting from Maillard reactions (Ferrer et al., 2005), very little is known about the volatile composition of infant formulas and their flavour characteristics.

In the present study, the volatile profiles of 13 infant formulas varying in brand, type (for different infant target groups) and physical form (powder/liquid) were characterised by proton transfer reaction-mass spectrometry (PTR-MS). The volatile compounds identified by gas chromatography–mass spectrometry (GC–MS). The PTR-MS data sets were related to the composition of the formulas.

2. Materials and methods

2.1. Samples

Thirteen different infant formulas were used in the study. They varied in brand, type (compositional characteristics depending on the target group) and physical form (Table 1). All 13 samples were analysed by PTR-MS and GC–MS analysis.

Table 1
Infant formula samples analysed by PTR-MS and GC–MS[a]

Brand	Type[a]			
	First	Hungrier	Follow-on	Soy
Aptamil	Powder/liquid	Powder	Powder	–
Cow & Gate	Powder/liquid	Powder	Powder	–
SMA	Powder	Powder/liquid	Powder	Powder

[a] The type 'first' was specified to be for normal infants for the age group 0–12 months, the type 'hungrier' for hungrier infants for the age group 0–12 months, the type 'follow-on' for all infants in the age group 6–24 months, and the type 'soy' for infants who do not tolerate cow's milk.

The powder formulas were prepared as directed on the packaging. For PTR-MS and GC–MS analysis 90 ml of previously boiled water at room temperature was placed in a 500 ml and 250 ml glass sample flask, respectively. Three scoops of the infant formula were added. The quantity of infant formula added varied with the brands: 90 ml of water was combined with 15 g of Aptamil, 14 g Cow & Gate and 13 g of SMA infant formula powder. Total volume was ca. 100 ml. The flask was closed with a cap and shaken manually. The formula was then allowed to equilibrate for 45 min at room temperature. For the liquid formulas the same volume (100 ml) was placed in the sample flask, and allowed to equilibrate for 45 min. For PTR-MS analysis, a magnetic stirrer was added prior to equilibration, and stirring was carried out from 20 min prior to the measurement. All samples were prepared in triplicate for PTR-MS analysis and in duplicate for GC–MS analysis.

2.2. Fingerprint PTR-MS analysis

The flask with the formula was connected to the PTR-MS transfer line. The sample was stirred continuously. The headspace was drawn at 20 ml/min, 15 ml/min of which was led into the PTR-MS (Ionicon Analytik, Innsbruck, Austria). The headspace of the sample was analysed by PTR-MS according to the method described by Lindinger, Hansel, and Jordan (1998), while employing a constant drift voltage of 600 V. The mass range 20–220 m/z was scanned for five subsequent cycles, the middle three cycles of which were used for calculations. Transmission of the ions through the quadrupole was considered according to the specification of the instrument. Background and transmission corrected spectra were averaged over three cycles for each individual sample replicate.

2.3. GC–MS analysis

Dynamic headspace analysis at room temperature was used to isolate the volatile compounds of the infant

formulas. The samples were prepared as described in Section 2.1. In addition, a blank sample without milk powder was prepared. The 100 ml of formula were prepared in a 250 ml glass flask. The formula was purged with purified nitrogen gas (100 ml/min) for 30 min and the volatile compounds trapped on Tenax TA (SGE, Kiln Farm Milton Keynes, UK) after condensing excess water vapour on a cold trap (−10 °C ethanol). The volatile compounds were identified by a combined GC (Varian Star 3400 CX, JVA Analytical Ltd., Dublin, Ireland) and MS (Varian Saturn 3, JVA Analytical Ltd.). Desorption of the volatile compounds from Tenax was performed by a thermal desorption (225 °C, 4 min)/cold trap (−100 °C) device (Tekmar Purge and Trap 3000 concentrator, JVA Analytical Ltd.). Through a heated transfer line, the volatile compounds were directed to the GC column (BPX5 capillary column, 60 m length, 0.32 mm i.d. and 1.0 μm film thickness, SGE). Helium (column flow rate 1.9 ml/min) was the carrier gas. The initial oven temperature was 40 °C for 4 min, and the temperature was subsequently programmed to 90 °C at 2 °C/min, further to 130 °C at 4 °C/min, and finally at 8 °C/min to 250 °C. Mass spectra were obtained with a 70 eV electron impact ionisation, while the mass spectrometer was scanning masses from m/z 25 to 400 at a speed of 2 scans/s. The volatile compounds were first identified by comparing their mass spectra with those of the NIST Mass Spectral Database and with those of pure compounds. Wherever possible, identities were confirmed by comparing their retention indices with either those of authentic compounds or those of published values (Kondjoyan & Berdague, 1996).

2.4. Statistical analysis

PTR-MS data were subjected to principal component analysis (PCA) and multivariate analysis of variance (MANOVA). PCA was also conducted on the compositional data of the formulas and separately on the combined PTR-MS and compositional data sets.

3. Results and discussion

3.1. Composition

Thirteen infant formulas, which differed in brand, type and physical form were selected (Table 1). The three brands examined were Aptamil, Cow & Gate and SMA. The types of formula were aimed at normal infants in the age group 0–12 months (first), at hungrier infants in the age group 0–12 months (hungrier), at infants in the age group 6–24 months (follow-on), and at infants who do not tolerate cow's milk well (soy). Two forms of the formula were studied: a powder and a liquid form. The composition of the major formula components (fat, protein, carbohydrates) of the 13 infant formula, as labelled, is presented in Table 2. A PCA was carried out on the compositional data, the plot of which is presented in Fig. 1. The PCA showed that the composition of the 'first' formula was very similar for the three brands. The compositions of the 'hungrier' and 'follow-on' equivalents were similar to each other, but varied per brand. For instance the Aptamil version of these two formulas were higher in carbohydrate content. The Cow & Gate powders were increased in protein content. The SMA formulas had also higher protein contents, but the extent was not the same for the 'hungrier' and 'follow-on' formula. The powder

Table 2
Gross composition of infant formulas (g/100 ml prepared product) according to label[a]

Sample	Fat	Protein	Whey	Casein	Carbohydrates
Aptamil					
First powder	3.6	1.4	0.8	0.6	7.3
First liquid	3.2	1.6	0.3	1.3	8.4
Hungrier powder	3.2	1.6	0.3	1.3	8.4
Follow-on powder	3.3	1.8	–[b]	–	9.2
Cow & Gate					
First powder	3.5	1.4	–	–	7.5
First liquid	3.5	1.4	–	–	7.5
Hungrier powder	3.3	1.7	–	–	7.8
Follow-on powder	3.4	1.8	–	–	8.1
SMA					
First powder	3.6	1.5	0.9	0.6	7.2
Hungrier powder	3.6	1.6	0.3	1.3	7.0
Hungrier liquid	3.6	1.6	0.3	1.3	7.0
Follow-on powder	3.0	2.2	–	–	7.8
Soy powder	3.6	1.8	–	–	6.9

[a] Samples are specified in Table 1.
[b] Not specified.

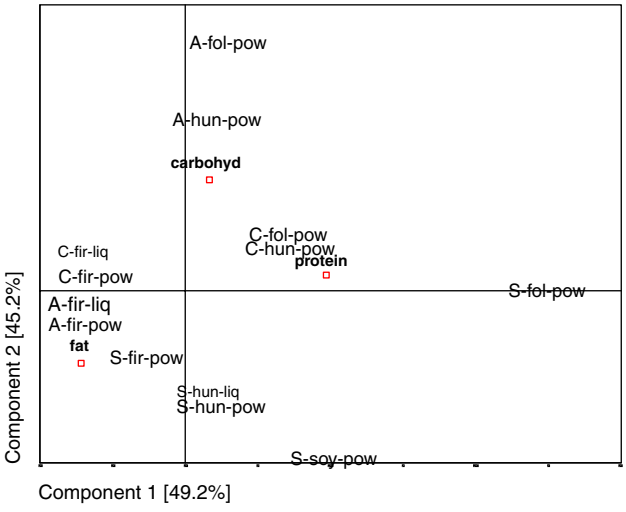

Fig. 1. First and second dimensions of principal component analysis on the compositional data of the 13 infant formulas. A, Aptamil; C, Cow & Gate; S, SMA; fir, first; hun, hungrier; fol, follow-on, pow, powder; and liq, liquid. Samples are specified in Tables 1 and 2.

and liquid forms of the same formula were identical in composition (after preparation).

3.2. Volatile compounds: PTR-MS

The 13 infant formulas were subjected to fingerprint PTR-MS analysis. The mass spectra of seven characteristic samples are presented in Fig. 2. They present samples for comparison of brands, type and physical form of the formula.

The mass spectral data were subjected to MANOVA, the results of which are presented in Table 3. It shows the importance of specific masses for discrimination between brands, type and physical form of the infant formulas. In total, 69 out of the 200 masses measured showed significant differences for at least one of the factors. Forty-two masses showed differences between brands (*m*/*z* 31, 33, 41, 42, 43, 44, 53, 55, 56, 57, 60, 67, 69, 70, 71, 72, 76, 77, 82, 83, 84, 85, 86, 87, 88, 93, 95, 97, 98, 99, 101, 102, 103, 111, 113, 115, 117, 118, 119, 125, 139 and 143). Forty masses showed differences between liquids and powders (*m*/*z* 24, 33, 43, 44, 45, 53, 55, 56, 57, 59, 60, 61, 62, 63, 64, 65, 67, 68, 73, 74, 75, 76, 77, 79, 80, 83, 84, 85, 86, 93, 95, 97, 99, 101, 102, 111, 113, 125, 139 and 143), and 14 masses showed differences between the type of formula (*m*/*z* 45, 49, 50, 56, 78, 80, 83, 84, 85, 93, 97. 111, 119 and 139).

PCA was carried out on the mass spectral data (Fig. 3). The data show that the formulas can be divided into three groups. SMA samples showed high positive scores on PC1. They were separated from both the Aptamil and Cow & Gate samples, which had high negative scores on the first PC. The powder and liquid samples were separated along PC2 independently of brand or type. High positive scores were observed for the liquid samples, and negative scores for the powder

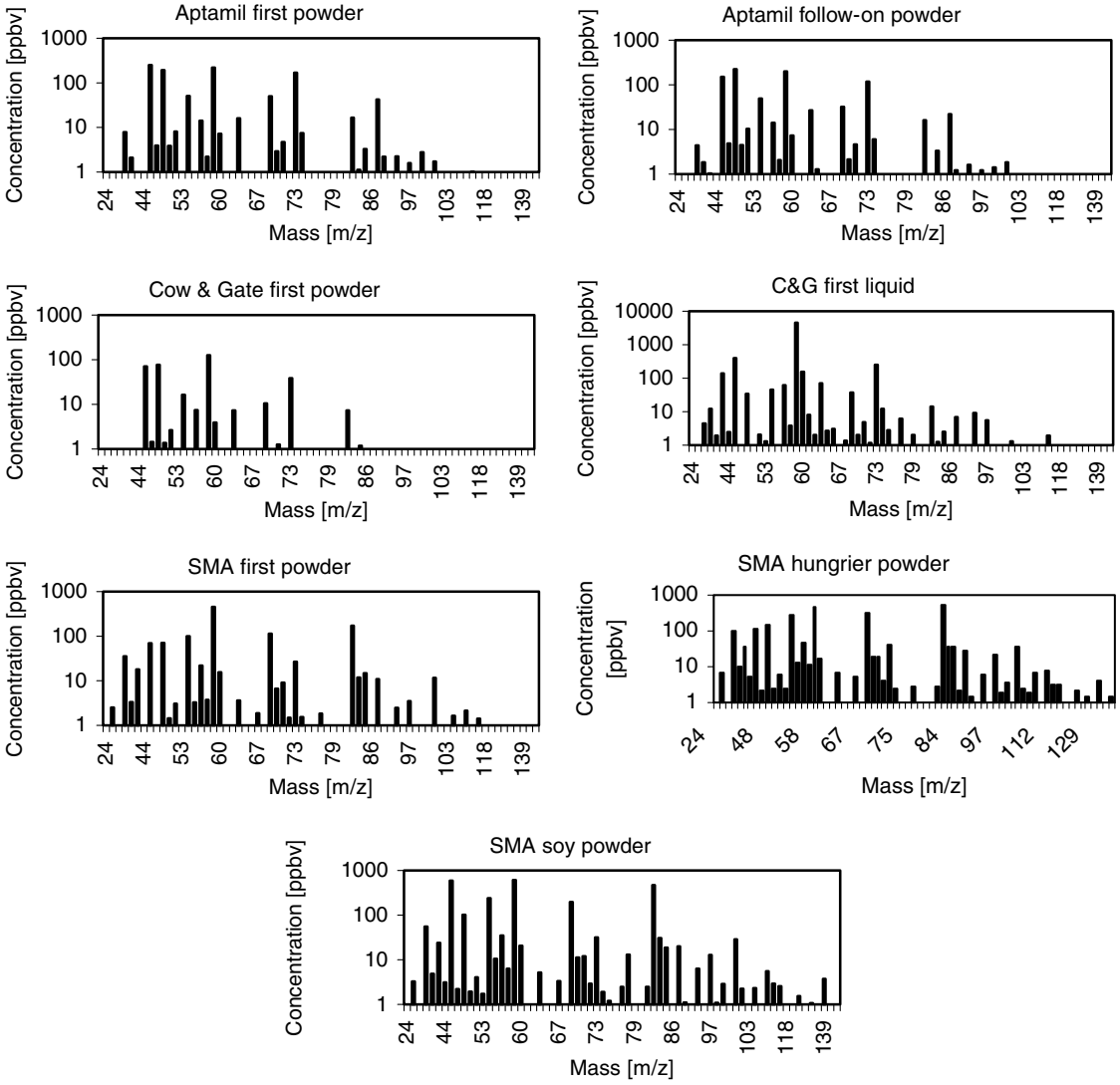

Fig. 2. Mass spectra of the volatile compounds of seven infant formulas obtained by proton transfer reaction-mass spectrometry. Ppb concentrations refer to concentrations in the headspace. Samples are specified in Tables 1 and 2.

Table 3
Analysis of variance results: probability levels (%) associated with *F*-values of the three factors brand, type and physical form

Mass (*m*/*z*)	Brand	Type	Form
24	84.1	21.6	**2.6**
31	**0.3**	60.1	90.2
33	**1.8**	67.6	**0.0**
41	**0.0**	9.6	34.9
42	**0.5**	65.6	15.2
43	**0.0**	30.7	**0.0**
44	**0.6**	77.5	**2.5**
45	68.2	**0.0**	**0.0**
48	12.1	19.0	55.1
49	9.5	**4.6**	10.4
50	9.5	**3.3**	9.7
51	12.6	6.6	21.3
53	**0.0**	49.1	**2.5**
55	**0.0**	5.9	**0.4**
56	**0.0**	**1.5**	**3.5**
57	**0.1**	67.7	**0.0**
58	0.0	25.7	16.3
59	0.0	96.0	**0.0**
60	**0.1**	96.6	**0.0**
61	22.5	31.8	**0.0**
62	58.9	41.6	**0.0**
63	13.2	94.3	**0.0**
64	16.4	80.1	**0.0**
65	6.3	75.1	**0.0**
67	**0.0**	10.4	**0.5**
68	18.0	50.9	**0.0**
69	**0.0**	11.3	9.7
70	**0.0**	13.8	10.6
71	**0.0**	8.2	11.1
72	**0.0**	33.6	97.3
73	5.7	84.6	**0.0**
74	8.3	86.1	**0.0**
75	10.5	24.0	**0.0**
76	**0.3**	59.9	**0.0**
77	**0.3**	77.6	**0.0**
78	96.3	**0.0**	14.4
79	39.0	9.5	**0.0**
80	75.4	**0.0**	**3.4**
82	**0.0**	20.1	8.6
83	**0.0**	**2.0**	**0.1**
84	**0.0**	**2.5**	**0.1**
85	**0.0**	**2.1**	**0.0**
86	**0.0**	10.6	**3.8**
87	**0.1**	41.3	56.4
88	**0.3**	89.5	13.4
93	**0.1**	**0.0**	**1.0**
95	**0.3**	49.6	**0.0**
96	12.1	31.7	21.2
97	**0.0**	**0.2**	**2.2**
98	**1.4**	34.3	24.2
99	**0.7**	16.8	**2.3**
100	9.4	73.8	86.5
101	**0.0**	14.3	**0.5**
102	**0.0**	14.9	**4.3**
103	**0.2**	61.3	92.4
111	**0.0**	**0.3**	**0.5**
112	6.1	70.1	89.6
113	**0.0**	2.9	**0.1**
115	**0.5**	10.7	33.3
117	**0.0**	53.5	17.3
118	**0.2**	22.5	20.1
119	**3.7**	**33.0**	25.7
125	**0.0**	17.4	**4.7**
128	8.5	24.6	36.7
129	39.4	90.3	49.2
130	38.5	81.1	71.2
139	**0.0**	**0.0**	**8.0**
140	19.4	73.0	69.5
143	**1.1**	34.8	**2.0**

Table 3 (*continued*)

In bold: significant probabilities at a 5% level.

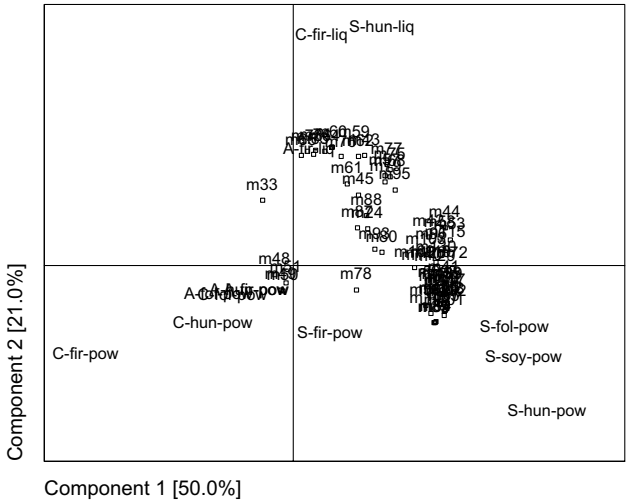

Fig. 3. First and second dimensions of principal component analysis on the mass spectral data of the infant formulas. A, Aptamil; C, Cow & Gate; S, SMA; fir, first; hun, hungrier; fol, follow-on, pow, powder; and liq, liquid. Samples are specified in Tables 1 and 2.

samples. Certain masses were related to the specific groups. For instance mass *m*/*z* 48, 49, 50 and 51 were related to the Aptamil and Cow & Gate powders. The concentration of volatiles in the headspace of the SMA powders was generally higher than for the other two brands. A large range of volatiles related to the SMA samples: (*m*/*z* 31, 41, 42, 44, 53, 56, 58, 67, 69, 70, 71, 72, 78, 80, 80, 82, 83, 84, 85, 86, 93, 96, 97, 98, 99, 100, 101, 102, 103, 111, 115, 117, 118, 119, 125, 128, 129, 130, 139, 140, 143). The characteristic masses for the liquid formulas were mass *m*/*z* 24, 33, 43, 45, 55, 57, 59, 60, 61, 62, 63, 64, 65, 68, 73, 74, 75, 76, 77, 79, 87, 88, and 95.

The mass spectral data were related to the compositional data (Fig. 4). PCA showed that samples high in carbohydrates were separated from those high in fat and protein content. For the latter high concentrations of a large range of masses was observed. Aptamil formula for hungrier babies and the Aptamil follow-on formula are the samples that are relatively high in carbohydrates (Fig. 1). For these samples generally low concentrations of volatiles were measured in the headspace.

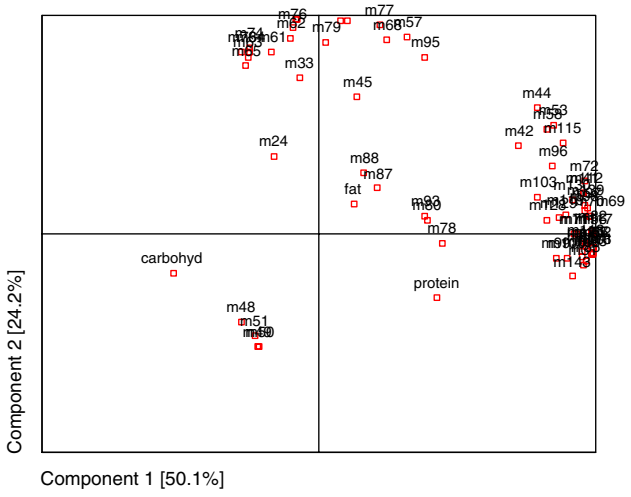

Fig. 4. First and second dimensions of principal component analysis on the mass spectral and compositional data of the infant formulas. A, Aptamil; C, Cow & Gate; S, SMA; fir, first; hun, hungrier; fol, follow-on, pow, powder; and liq, liquid. Samples are specified in Tables 1 and 2.

One related study was found in the literature. This study evaluates a MS-based electronic nose for its ability to differentiate various infant formula powders based on changes of their volatile composition upon storage (Fenaille et al., 2003). In this study, after multivariate treatment, the MS data resulted in differentiation of the infant formulas over a 4 weeks storage test. Although the test was easy-to-use and fast, its disadvantage was that the compounds could not be identified and quantified. Although with this technique discriminating ions could be selected, it was not possible to further relate these ions to a characteristic compound because of the high ion fragmentation classically obtained in EI ionisation mode. The type of ionisation is the main difference between the MS-based electronic nose and PTR-MS. In PTR-MS analysis, soft ionisation is applied which reduces fragmentation considerably. For that reason, ions measured in PTR-MS are often the parent ions (M^{+1}). Because of the soft ionisation, the measured ions can often be related to characteristic compounds.

3.3. Volatile compounds: GC–MS

The volatile compounds of the 13 infant formulas were identified by GC–MS. The analysis resulted in identification of 28 compounds. They are listed in Table 4 together with their expected parent or fragment ion in PTR-MS analysis. Aldehydes, ketones, alcohols, sulfur compounds, and acids were present among the compounds identified. In very few studies the volatile compounds of infant formulas have been identified. Romeu-Nadal et al. (2004) identified and quantified propanal, pentanal and hexanal in non-oxidised and oxidised powder infant formula samples by comparison

Table 4
Volatile compounds identified in the headspace of infant formulas by gas chromatography–mass spectrometry analysis, their retention indices (RI), and expected parent mass or fragment in proton transfer reaction mass spectrometry analysis

Compound	RI	Expected major mass fragment
Acetic acid	<600	61[a]
Acetone	<600	59[a]
2-Methylpropanal	<600	55[c]
Dimethyl sulfide	<600	63[a]
2-Butenal	600	71[c]
2-Butanone	600	73[b]
Butanal	614	55[b]
2-Methyl-3-buten-2-ol	629	69[a]
3-Methylbutanal	644	69[a]
3-Methyl-3-buten-1-ol	671	69[a]
2-Methylbutanal	682	87[a]
1-Penten-3-ol	689	–[d]
3-Methyl-2-butanone	691	–
Ethyl cyclopentane	696	–
Pentanal	705	69[b]
Methyl propanoate	716	75[b]
3-Methyl-1-butanol	741	43[c]
3,4-Dihydro-2*H*-pyran	741	–
2-Methyl-1-butanol	747	43[c]
trans-2-Pentenal	751	67
Dimethyl disulfide	756	95[a]
1-Octene	767	–
Hexanal	812	83[b]
cis-3-Octen-1-ol	838	69[c]
trans-3-Nonene	850	–
Ethyl benzene	871	–
1-Hexanol	878	43[b]
Heptanal	914	97[b]

[a] Fragmentation patterns reported by Yeretzian et al. (2003).
[b] Fragmentation patterns reported by Buhr et al. (2002).
[c] Fragmentation expected from patterns of homologous compounds reported by Yeretzian et al. (2003) and Buhr et al. (2002).
[d] Fragmentation pattern unknown.

of retention times of the compounds with those of standards. During storage, the equilibrium headspace concentrations of the compounds were followed. Although initially already present, the concentrations of the compounds had increased 4- to 10-fold their original concentrations after storage for 4 weeks. In the present study, both pentanal and hexanal were identified. The aldehydes pentanal, hexanal, heptanal and nonanal are common indicators of oxidative deterioration, also for other types of milk powder products (Ulberth & Roubicek, 1995). Fenaille et al. (2003) identified 16 volatile compounds in the headspace of infant formulas by solid phase microextraction gas chromatography. Five of these compounds, i.e., 2-butanone, pentanal, 2-pentenal, hexanal and heptanal, have been identified in the present study as well.

Some of the volatile compounds identified in the infant formulas show similarity with those identified in other types of milk powders. For instance, 2-methyl-3-buten-2-ol, hexanal and acetic acid were also identified in skim milk powder (Shiratsuchi, Shimoda, Imayoshi,

Table 5
Ranks of mass fragments highest in intensity (1 = highest) in proton transfer reaction mass spectrometry analysis for 13 infant formulas and related compounds based on gas chromatography–mass spectrometry analysis and expected fragmentation patterns (Yeretzian et al., 2003; Buhr et al., 2002)[a]

Sample	Methylbutanal, hexanal	Fragment aldehydes		Butanal, methyl propanal, fragment aldehydes	Acetone		Dimethyl sulfide	Methylbutenol, 3-methylbutanal, pentanal	2-Butanone	Hexanal	2-Methylbutanal
	m/z 43	*m/z* 45	*m/z* 49	*m/z* 55	*m/z* 59	*m/z* 60	*m/z* 63	*m/z* 69	*m/z* 73	*m/z* 83	*m/z* 87
Aptamil											
First powder		1	3	5	2				4		
First liquid		2			1		5	3	4		
Hungrier powder		3	1	5	2				4		
Follow-on powder		3	1	5	2				4		
Cow & Gate											
First powder		3	2	5	1				4		
First liquid	5	2			1	4			3		
Hungrier powder		2	1	5	4				3		
Follow-on powder		2	1	5	3				4		
SMA											
First powder			5	4	1			3		2	
Hungrier powder			5	4	2			3		1	
Hungrier liquid		3	5		1	4			2		
Follow-on powder		4	5	3	1					2	
Soy powder		2		4	1			5		3	

[a] Samples are specified in Tables 1 and 2.

Noda, & Osajima, 1994). Acetone, 2-methylpropanal, 2-butanone, 2- and 3-methylbutanal and acetic acid have been detected in skim milk powders by Turner, Linforth, and Taylor (2002). Acetic acid, pentanal, hexanal, heptanal and dimethyl disulfide have been determined in whey protein concentrates (Le Quach, Dong Chen, & Stevenson, 1999).

3.4. Relating PTR-MS and GC–MS analysis

For each of 13 infant formulas the five most abundant ions in PTR-MS were ranked one to five (Table 5). Across the samples, eleven ions were present most abundantly (*m*/*z* 43, 45, 49, 55, 59, 60, 63, 69, 73, 83 and 87). The ions were related to volatile compounds identified in GC–MS analysis (Table 5). Some of the aldehydes, acetone and 2-butanone are present at high concentrations in most samples. Some compounds are more specific for certain samples. For instance, 2-butanone is one of the most abundant compounds in the headspace of the Aptamil and Cow & Gate samples. Hexanal is a compound high in concentration in the headspace of the SMA samples, whereas it is relatively less abundant in the samples of the two other brands. Mass *m*/*z* 49 and *m*/*z* 55 (butanal, methyl propanal and/or a fragment of other aldehydes) are characteristic for the liquid samples. There are usually also other abundant compounds present in the headspace of the liquid samples, but the type of compound varies per brand.

4. Conclusions

PTR-MS analysis allowed characterisation of the volatile profiles of 13 infant formulas. Different brands and physical forms resulted in different mass spectra, which could be related to characteristic volatile compounds.

References

Albalá-Hurtado, S., Veaciana-Nogués, M. T., Mariné-Font, A., & Vidal-Carou, M. C. (1998). Changes in furfural compounds during storage of infant milks. *Journal of Agricultural and Food Chemistry, 46*, 2998–3003.

Buhr, K., van Ruth, S., & Delahunty, C. (2002). Analysis of volatile flavour compounds by proton transfer reaction-mass spectrometry: fragmentation patterns and discrimination between isobaric and isomeric compounds. *International Journal of Mass Spectrometry, 221*, 1–7.

Fenaille, F., Visani, P., Fumeaux, R., Milo, C., & Guy, P. A. (2003). Comparison of mass spectrometry-based electronic nose and solid phase microextration gas chromatography–mass spectrometry technique to assess infant formula oxidation. *Journal of Agricultural and Food Chemistry, 51*, 2790–2796.

Ferrer, E., Alegría, A., Farré, R., Abellán, P., & Romero, F. (2005). High-performance liquid chromatographic determination of furfural compounds in infant formulas during full shelf-life. *Food Chemistry, 89*, 639–645.

Kondjoyan, N., Berdague, J.-L. (1996). A compilation of relative retention indices for the analysis of aromatic compounds (1st ed.). Laboratoire Flaveur, Station de Recherches sur la Viande, Inra de Theix, 63122 Saint Genes Champanelle, France. 234 p.

Le Quach, M., Dong Chen, X., & Stevenson, R. J. (1999). Headspace sampling of whey protein concentrate solutions using solid-phase microextraction. *Food Research International, 31*, 371–379.

Lindinger, W., Hansel, A., & Jordan, A. (1998). On-line monitoring of volatile organic compounds at pptv levels by means of proton transfer reaction-mass spectrometry (PTR-MS): Medical applications, food control and environmental research. *Journal of Mass Spectrometry and Ion Processes, 173*, 191–241.

Menella, J. A., & Beauchamp, G. K. (1996). Developmental changes in the infants' acceptance of protein-hydrolysate formula and its relation to mothers' eating habits. *Journal of Developmental and Behavioral Pediatrics, 17*, 386–391.

Menella, J. A., & Beauchamp, G. K. (1999). Experience with a flavor in mother's milk modifies the infant's acceptance of flavored cereal. *Developmental Psychobiology, 35*, 197–203.

Menella, J. A., & Beauchamp, G. K. (2002). Flavor experiences during formula feeding are related to preferences during childhood. *Early Human Development, 68*, 71–82.

Menella, J. A., Jagnow, C., & Beauchamp, G. K. (2001). Pre- and postnatal flavor learning by human infants. *Pediatrics, 107*, e88.

Romeu-Nadal, M., Castellote, A. I., & López-Sabater, M. C. (2004). Headspace gas chromatographic method for determining volatile compounds in infant formulas. *Journal of Chromatography A, 1046*, 235–239.

Shiratsuchi, H., Shimoda, M., Imayoshi, K., Noda, K., & Osajima, Y. (1994). Volatile flavor compounds in spray-dried skim milk powder. *Journal of Agricultural and Food Chemistry, 42*, 984–988.

Turner, J. A., Linforth, R. S. T., & Taylor, A. J. (2002). Real-time monitoring of thermal flavor generation in skim milk powder using atmospheric pressure chemical ionization mass spectrometry. *Journal of Agricultural and Food Chemistry, 50*, 5400–5405.

Ulberth, F., & Roubicek, D. (1995). Monitoring of oxidative deterioration of milk powder by headspace gas chromatography. *International Dairy Journal, 5*, 523–531.

Yeretzian, C., Jordan, A., & Lindinger, W. (2003). Analysing the headspace of coffee by proton-transfer-reaction mass-spectrometry. *International Journal of Mass Spectrometry, 223–224*, 115–139.