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Characterisation of fresh bread flavour: Relationships between sensory characteristics and volatile composition

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ABSTRACT

The sensory properties and volatile composition of bread flavour were measured to allow improved understanding of perceived bread freshness. Twenty bread varieties consisting of specialty breads ($n = 10$) and commercial breads ($n = 10$) were evaluated by descriptive sensory analysis, and volatile composition of all breads was measured by proton transfer reaction mass spectrometry (PTR-MS). The specialty breads ($n = 10$) studied had been evaluated by consumers, and perceived freshness was known. All sensory attributes and 33 mass ions representative of the PTR-MS spectra significantly ($p < 0.05$) distinguished between the different breads. Partial least squares regression (PLSR) was used to model and predict sensory profiles as a function of volatile composition for all breads. In addition, a separate model that related volatile composition to known consumer freshness of the 10 specialty breads was created. For each model, accuracy was validated by comparing the differences between predicted and actual, sensory and freshness intensities.

1. Introduction

Fresh bread flavour is central to consumer acceptability and product recognition. The flavour perception perceived while eating involves complex interactions between sensory sensations of olfaction, taste and trigeminal stimuli (Lawless & Heymann, 1999). From this aspect, sensory descriptive analysis has been commonly applied to measure the odour and flavour impressions of food (Meilgaard, Civille, & Carr, 1999; Stone & Sidel, 2004). Among the various intrinsic properties of bread, volatile flavour compounds play a key role in the perception of fresh bread flavour. However, the perceived fresh bread flavour often relies on the type of bread, ingredients, method of production and shelf life.

Considerable research has focused on describing bread flavour using descriptive sensory analysis (Caul & Vaden, 1972; Chang & Chambers, 1992; Lotong, Chambers, & Chambers, 1999; Shogren, Mohamed, & Carriere, 2003). Additionally, several studies have applied descriptive sensory analysis to describe consumer perceptions of different bread varieties (Hersleth, Berggren, Westad, & Martens, 2005), effects of bread produced from different wheat grains (Annett, Spaner, & Wismer, 2007), influences of processing (Heinio, Liukkonen, Katina, Myllymaki, & Poutanen, 2003), as well as influences of farming system, harvest, milling and baking techniques (Kihberg, Johansson, Kohler, & Risvik, 2004; Kihlberg, Ostrom, Jahansson, & Risvik, 2006). Heenan, Dufour, Hamid, Harvey, and Delahunty (2008) showed that sensory characteristics from different bread varieties influenced consumer perceptions of freshness and demonstrated that by relating subjective consumer freshness judgements to descriptive sensory attributes from a trained panel, an objective understanding of bread freshness could be obtained.

Research has been carried out on the flavour of fresh bread by identifying key odour active volatile compounds (Chang, Seitz, & Chambers, 1995; Kirchhoff & Schieberle, 2001; Schieberle & Grosch, 1992; Seitz, Chung, & Rengarajan, 1998; Zehentbauer & Grosch, 1998a, 1998b). According to Schieberle and Grosch (1992), the loss of fresh bread flavour results from specific compound volatility, where important odourants rapidly decreased during storage, whilst less desirable odourants characterised from lipid oxidation remained relatively unchanged.

Sensory and instrumental volatile analysis has shown that different fermentation conditions and the amount of yeast, changed the flavour profile for crust aroma of baguettes (Zehentbauer & Grosch, 1998a, 1998b). Other studies have reported distinct differences between the headspace volatile composition of commercially made breads that included white sandwich, Irish oatmeal, soft rye, hearty rye, sourdough, home-like white and onion-basil (Seitz et al., 1998), and between breads produced from different

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wheat varieties (Chang et al., 1995). More recently it was suggested that consumer preferences for commercial wheat type baguettes could be related to volatile compounds (Quilez, Ruiz, & Romero, 2006).

More than 300 volatile compounds have been identified from bread (Pozo-Bayon, Guichard, & Cayot, 2006). Considering the many varieties of bread that are available and the vast amount of volatile compounds that exist, correlation of sensory character with volatile composition is difficult. However, analysis of spectral data from a rapid sensitive instrumental technique such as proton transfer reaction mass spectrometry (PTR-MS) has demonstrated the ability to model relationships between sensory attributes (odour/flavour) and volatile composition (Biasioli et al., 2006). PTR-MS provides the ability to measure the volatile composition of food without pre-treatment enabling many samples to be analysed in a short period of time (Lindinger, Hansel, & Jordan, 1998). To date, this analytical technique coupled with multivariate statistical analysis has been used successfully to characterise and differentiate the volatile composition of cheese (Aprea et al., 2007b; Biasioli et al., 2006; Boscaini, van Ruth, Biasioli, Gasperi, & Mark, 2003; Gasperi et al., 2001), custard desserts (van Ruth, De Witte, & Uriarte, 2004), infant formulas (van Ruth, Floris, & Fayoux, 2006), truffles (Aprea et al., 2007a), olive oil (Aprea et al., 2006), whey (Gallardo-Escamilla, Kelly, & Delahunty, 2005; Gallardo-Escamilla, Kelly, & Delahunty, 2007), orange juice (Biasioli et al., 2003), meat (Mayr, Margesin, Schinner, & Mark 2003b; Mayr et al., 2003a), and whole strawberries (Granitto et al., 2007). More recently, Lindinger et al. (2008) developed a predictive model for flavour attributes of espresso coffee that linked PTR-MS measurements and sensory profiling data. This approach enabled a rapid characterisation of flavour for different espressos. There has been no studies that have investigated sensory characteristics and volatile composition of different bread varieties using PTR-MS analysis. Hence, the opportunity remains to model and predict sensory attributes of different bread varieties using measurements from a rapid headspace PTR-MS technique.

The present investigation was carried out to characterise fresh bread flavour by relating sensory characteristics defined by odour and flavour attributes to volatile composition measured by PTR-MS, of different bread varieties. In addition, known consumer freshness perceptions from 10 specialty breads (Heenan et al., 2008) were related to their volatile composition. Relationships were determined using partial least squares regression (PLSR) modelling (Martens & Martens, 1986). The predictive ability of multivariate models for determining sensory attributes and overall consumer freshness perceptions from volatile composition was validated and tested, using a subset of commercially available bread types. In this study, relating volatile data from PTR-MS with sensory analysis and known consumer freshness perceptions offered a new and rapid technique to characterise and predict fresh bread flavour.

2. Materials and methods

2.1. Bread samples

Twenty breads were selected to represent a range of different breads that consisted of both specialty ($n = 10$) and commercially branded ($n = 10$) varieties currently available in the New Zealand market (Table 1). For descriptive analysis all samples were produced and purchased from local bakeries and evaluated within 4 h from baking on four separate days. Duplicates of each sample, each from a different batch were presented in two sets of five on separate days. Thus each panellist received 10 samples per session. For each session, three loaves of each bread type (i.e. multigrain, foccacia, white, sourdough, pugliese, Ciabatta, rye, commercial mixed grain, commercial Swiss rye, commercial wheat, commercial mixed grain, commercial whole wheat, commercial oat bran) and six individual bread types (i.e. croissant, bagel, brioche, English muffin, panini, baguettes) were produced and baked on a daily basis. A separate batch of breads was produced and baked for PTR-MS analysis, and were analysed in triplicate within a single day. Similar to descriptive analysis, three loaves of each bread type and six individual bread types from the same batch were produced and baked on the day of testing. In terms of freshness, time of baking was carefully chosen to ensure that all breads were equally fresh at the point of evaluation.

From a prior study undertaken by the same authors (Heenan et al., 2008), mean consumer freshness scores of the 10 specialty breads was known (Table 1). Due to commercial sensitivity, the branded bread ($n = 10$) varieties were labelled BR1–BR10.

2.2. Descriptive sensory analysis

A panel of 11 assessors (9 females, 2 males aged between 24 and 55 years) were trained following international standards (ISO, 1993). The trained panel used a descriptive vocabulary that encompassed 18 attributes for evaluating the bread odour (i.e. dairy, yeasty, flour, grain, musty, nutty, malty, toasted) flavour (i.e. sweet, salty, sour, bitter, buttery, oily, seedy) and after-flavour (i.e. bitter, sour, toasted). Attribute definitions for odour, flavour and after-flavour are described in Heenan et al. (2008). A 50 g portion of each sample, including the crust and crumb, was presented to assessors in 3-digit coded glasses covered with a glass cover, in a balanced ordered design (MacFie & Bratchell, 1989). Assessments were carried out in individual booths under white light at room temperature. Two and 15 min intervals were allowed between each sample and each set of five samples, respectively. For evaluation, each assessor was provided with filtered water and un-salted crackers and asked to cleanse their palate between tastings. In addition, assessors received a list of attributes that included definitions to aid in their assessments. Sample attributes were scored on unstructured 100 mm line scales labelled from low at 5 mm to high at 95 mm intervals. For each attribute, ratings on the unstructured line scale were measured geometrically to produce intensity values.

2.3. Volatile composition determination using PTR-MS

The volatile composition of each bread sample was measured in triplicate using a high sensitivity PTR-MS instrument (Ionicon Analytik, Innsbruck, Austria). All measurements were carried out under drift tube conditions of 120–130 Td (Td = Townsend; 1 Td = 10^{-17} V cm^2 mol^{-1}) over a mass range of $m/z = 20$ to $m/z = 180$ and a dwell time of 0.2 s mass^{-1}, giving a cycle time of 32 s. Each bread type was cut into approximately $30 \times 30 \times 20$ mm cubes and separately weighed (100 g) into 1 l glass bottles (Schott Duran bottles, Germany) and allowed to equilibrate at room temperature (~20 °C) for 1 h. Bottles were connected to the PTR-MS inlet flow that was heated to 80 °C via Teflon (0.25 mm) tubing and headspace air was sampled at a flow rate of 50 ml/min. The headspace air was replaced by an equal flow of pure air (BOC, New Zealand; purity; oxygen 21.999%, nitrogen 77.999%). Masses were analysed in a quadrupole mass spectrometer and detected as ion counts per second (cps) by a secondary electron multiplier (SEM). Sample measurements were performed in six cycles resulting in an analysis time of 3.2 min. The mean of cycles 2–6 were represented in further analysis. Background air scans of five cycles were conducted from an empty bottle before each sample measurement and the mean signal was subtracted from the sample spectra (Aprea et al., 2007b). Mass ion intensities

Table 1
Bread products sampled and listed ingredients.

Sample	Consumer perceived freshness[a]	Ingredients
Speciality breads		
Multigrain	38.0	High Gluten Flour, Wholemeal Flour, Coarse Rye, Kibbled Rye, Buck Wheat Goats, Linseeds, Burghal Wheat, Gluten Flour, Yeast, Milk, Water, Sugar, Salt, Butter
Croissants	67.6	High Gluten Flour, Yeast, Milk, Water, Sugar, Salt, Butter, Egg
Bagel	50.9	High Gluten Flour, Yeast, Milk, Water, Sugar, Salt, Butter
Foccacia	69.1	High Gluten Flour, Yeast, Milk, Water, Sugar, Salt, Olive Oil, Egg
White	53.9	High Gluten Flour, Yeast, Milk, Water, Sugar, Salt, Butter, Egg
Sourdough Loaf	37.1	High Gluten Flour, Wholemeal Flour, Yeast, Wild Yeast, Milk, Water, Sugar, Salt, Butter, Egg
Brioche	57.0	High Gluten Flour, Yeast, Milk, Salt, Sugar, Butter, Egg
Pugliese	55.9	High Gluten Flour, Drum Flour, Yeast, Milk, Water, Sugar, Salt, Butter
Ciabatta	54.2	High Gluten Flour, Yeast, Milk, Water, Sugar, Salt, Butter
Rye	65.1	High Gluten Flour, Wholemeal Flour, Refined Rye Flour, Yeast, Milk, Water, Sugar, Salt, Butter, Molasses
Commercial bread brands		
BR1 (Whole grain)	–	Water, Wheat Flour, Kibbled Soya Beans, Linseeds, Mixed Grains, Wheat, Rye, Wheat Gluten, Vegetable Oil, Yeast, Salt, Milk Solids, Vinegar
BR2 (English muffin)	–	Wheat Flour, Water, Yeast, Sugar, Wheat Gluten, Salt, Soy Flour,
BR3 (Swiss rye)	–	Water, Wholemeal Wheat Flour, Kibbled Rye, Wheat Flour, Gluten, Vinegar, Vegetable Oil, Milk Solids, Yeast, Cultured Whey, Acidity Regulator
BR4 (White)	–	Wheat Flour, Yeast, Salt, Vegetable Oil, Soy Flour, Sugar
BR5 (Mixed grain)	–	Water, Wheat Flour, Mixed Grains, Wheat, Rye, Skim Milk Powder, Wheat Gluten, Salt, Vinegar, Yeast.
BR6 (Panini)	–	Wheat Flour, Water, Canola Oil, Olive Oil, Yeast, Sugar, Salt, Soy Flour
BR7 (Rye)	–	Water, Wheat Flour, Mixed Grains, Wheat, Rye, Kibbled Spelt, Flaxseed, Wheat Gluten, Kibbled Corn, Canola Oil, Sugar, Yeast, Salt, Milk Solids, Vinegar, Malted Barley
BR8 (Whole wheat)	–	Wheat Flour, Kibbled Rye, Oat Bran, Yeast, Water, Wheat Gluten, Salt, Canola Oil, Soy Flour
BR9 (Oat bran)	–	Wheat Flour, Water, Oat Bran, Wheat Bran, Yeast, Sugar, Soy Flour, Gluten, Salt, Vegetable Oil
BR10 (Baguette)	–	Wheat Flour, Water, Gluten, Soy Flour, Malt Flour, Yeast, Salt, Sugar

[a] Mean values of freshness scores as reported in Heenan et al. (2008).

were converted to concentration (pbbv) according to Lindinger et al. (1998). Sample measurements were conducted over a 5 h time frame from the first to the last sample. The order of sample and triplicate measurements were randomised to account for possible changes in products volatile composition over time.

2.4. Data analysis

For each sensory attribute measured, a two-way analysis of variance (ANOVA) with interaction was applied using SPSS 12.0.1 (SPSS Inc., Chicago, USA), to monitor assessor performance for reproducibility and determine attributes that discriminated among samples. Factors were set as fixed for *bread type* and *replicate*, and random for *assessor* (Lundahl, 1990; Lundahl & McDaniel, 1988). In addition, triplicate volatile mass ion concentrations from PTR-MS measurements were analysed by one-way ANOVA. Attributes and volatile compounds that did not significantly discriminate between bread types were not included in further analysis. This reduction of insignificant attributes and compounds ensured extraction of the most relevant variables for more robust correlations to be investigated. Post-hoc Tukey honestly significant difference (HSD) testing ($p < 0.05$) was carried out on each data set (i.e. sensory and volatile), to determine significant differences between pairs of samples for sensory attributes and mass compounds.

Both sensory and volatile compound data sets were standardised (1/standard deviation) and analysed by PCA using the Unscrambler version 9.1 software (CAMO, AS, N-7041, Trondheim, Norway). The purpose of standardisation in this case was to allow for all variables to give equal influence to the PCA model, regardless of their original variance. In this study, standardisation enabled direct comparisons to be made between the two data sets despite differences in their numerical range (Westad, Hersleth, Lea, & Martens, 2003). One-way ANOVA was carried out on PCA scores for both data sets to determine the number of principal components (PCs) that significantly ($p < 0.05$) discriminated breads using both sensory attributes and volatile compounds of the different bread types prior to averaging across replicates.

Partial least squares regression type 1 (PLSR1) was used to investigate relationships between sensory attributes, known consumer freshness perceptions and volatile composition (Martens & H., 1986). To model sensory attributes as a function of volatile composition, 15 out of 20 bread types that represented the sensory and volatile distribution of the breads tested were selected. Model performance was tested (validated) by comparing actual and predicted sensory attribute intensity scores for the remaining five commercial bread types not used in the construction of models. In addition and separately, known freshness evaluations from the 10 specialty breads (Heenan et al., 2008) were related to volatile composition, and predictions of freshness were made for the 10 commercial breads not evaluated by consumers. PLSR1 was applied to create separate models relating volatile components (X-variables) to sensory attributes and freshness perceptions (Y-variables) one at a time. Full cross validation was used to select the optimum number of PLS factors for predicting the Y-data sets. The calibration and validation coefficients that express model fit in X and Y, and ability to predict new data were monitored. For each model the regression coefficients (β-coefficients) were graphed to determine the contribution of each X-variable in predicting Y-variables. Variables that contributed little and/or displayed high levels of uncertainty estimates were identified using the jack-knife method (Martens, Bredie, & Martens, 2000; Martens & Martens, 2000). Subsequent models were recalibrated with non contributing X-variables removed and final PLSR models were selected based on the root mean square error of prediction (RMSEP). The RMSEP represents the average prediction error expected for new samples based on the same units of measurements as the original response variables (sensory attributes on a scale from 0 to 100 mm, and freshness on a scale from 0 to 150 mm). In addition, RMSEP was used to study the relationship between modelling error and estimation error to determine the optimum number of PCs to be used.

PLSR models were used to predict the sensory attributes and freshness intensities for all bread types, and for the five and 10 breads that were excluded when building the models. Comparisons between actual sensory intensity and known freshness, and predicted sensory intensity and freshness for breads were represented. To examine the linear relationship between the actual and predicted values, Pearson correlation coefficients were calculated, thus providing a further means of model validation.

3. Results and discussion

3.1. Descriptive sensory analysis

All sensory attributes used in descriptive analysis significantly discriminated ($p < 0.05$) between the bread types tested. ANOVA of PC scores, based on replicate evaluations showed that the first five PCs significantly discriminated ($p < 0.05$) between the samples, and accounted for 34%, 18%, 16%, 10% and 8% of the experimental variance, respectively. The PCA clearly showed differences in the sensory profile between the bread types and illustrated relationships between sensory attributes. The first four PCs were represented in PCA biplots (Fig. 1a and b). Variance across PC 1 was explained by differences between the sensory characteristics of croissant, rye bread, and brioche along the positive axis, and commercial breads BR5 (mixed grain), BR3 (Swiss rye) and multigrain along the negative axis. Croissant and rye bread, described by sensory characteristics of "dairy", "malty" odour and a "sweet", "floury" flavour were considered to be fresher by consumers (Table 1). Croissant and rye bread were produced from standard high gluten wheat flour. According to Martinez-Anaya (1996), the carbohydrate content of standard wheat flour is easily broken down into simple sugars during bread production, which influences the occurrence of sweet, caramel and malty flavours during baking. Subsequently, thermal reactions associated with freshly baked bread, include caramelization and non-enzymatic browning, which generate important volatile compounds such as furans, pyrazines, pyridines, pyrol and Strecker aldehydes (Grosch & Schieberle, 1997; Pozo-Bayon et al., 2006).

In contrast, BR5 (mixed grain), BR3 (Swiss rye) and multigrain were described as "musty", "grainy", "nutty" in odour, and "sour" and "seedy" in flavour. Sensory characteristics of "musty", and "sour" have been reported to influence the degree of freshness for different Finish rye breads (Hellenmann, Tuorila, Salovaara, & Tarkkonen, 1987), while "grainy" and "nutty" characteristics have been shown to differentiate different types of sourdough bread (Lotong et al., 1999) and wheat soy flour breads (Shogren et al., 2003), respectively. BR5 (mixed grain), BR3 (Swiss rye) and multigrain all contained mixed whole grains, wholemeal flour and kibbled rye (Table 1). The outer bran layer of whole grains has been shown to influence the perceived grainy cereal and bitter flavours of bread (Chang & Chambers, 1992; Heinio et al., 2003).

Along the positive axis, PC2 was described by the attributes "yeasty", "oily" odour and "salty", "buttery", "dairy" flavour, which were present in foccacia bread. Along the negative axis of PC2 "toasted" odour was present in commercial breads, BR9 (oat bran) and BR10 (baguette). The "oily" flavour of foccacia bread could be explained by its olive oil content. Additional PCs revealed further sensory differences between the breads (Fig. 1b). PC3 distinguished differences between the "sweet" flavour of rye bread and "sour" after-flavour of bagel. PC4 showed that ciabatta, foccacia and commercial bread BR10 (baguette) were similar in terms of "floury" odour and "bitter" flavour, whilst croissant, multigrain and brioche were similar in terms of "nutty" odour.

3.2. Headspace volatile composition of bread

One-way ANOVA identified 33 mass ions (m/z) 27, 29, 33, 43, 45, 47, 55, 59, 61, 63, 65, 69, 73, 75, 79, 83, 85, 87, 89, 91, 93, 97, 98, 101, 103, 105, 107, 111, 113, 117, 121, 125, 129) out of 160

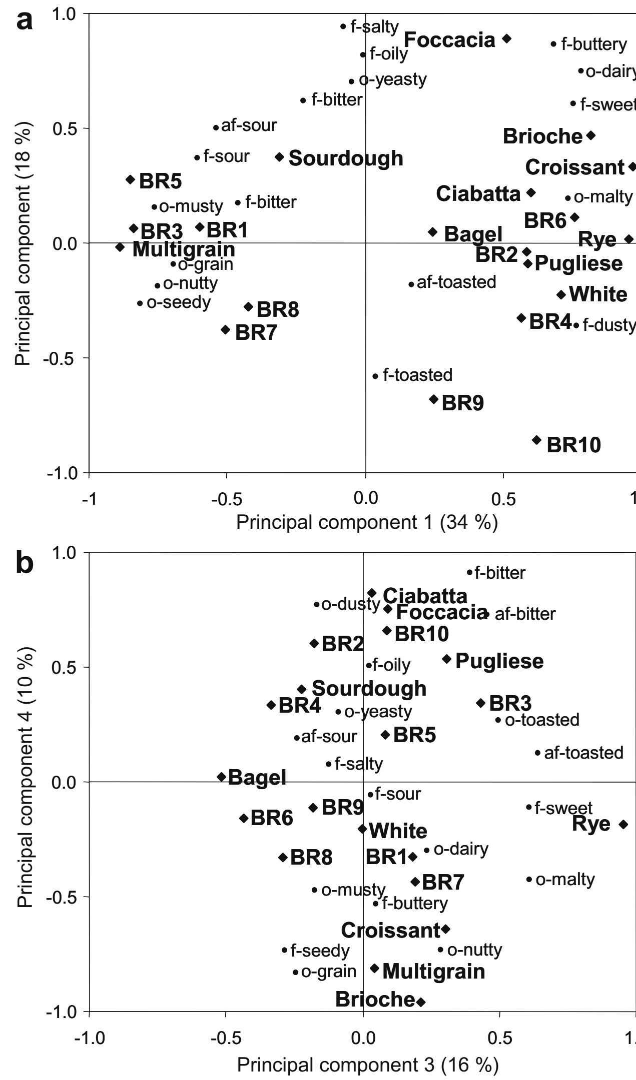

Fig. 1. Results of Principal Component Analysis biplot showing the sensory attributes of the specialty breads and commercial breads (BR1–BR10) for the first two components.

masses measured that significantly ($p < 0.05$) discriminated between the bread types. In principal, a PTR-MS spectrum constitutes, a 'volatile-fingerprint' for an individual sample. For example, fresh samples of sourdough and brioche could be distinguished based on their headspace mass spectra (Fig. 2). Brioche was shown to have relatively high concentrations of the masses m/z 43, 87, 89 and 113, whilst sourdough comprised high concentrations of masses m/z 47, 75, 103, 105, 107, 125, 129. PCA illustrated product differences by volatile composition, on the basis of mass ions that discriminated between the bread types (Fig. 3a and b). ANOVA of PC scores, based on triplicate analyses showed that the first five PCs significantly ($p < 0.05$) discriminated between the samples, and accounted for 31%, 22%, 13%, 10% and 5% of the experimental variance, respectively. Along the positive axis, PC1 was described by the masses m/z 55, 69, 103, 107 and 125, present in relative high concentrations in sourdough and commercial breads BR3 (Swiss rye) and BR8 (whole wheat). Along the negative axis, masses m/z 83, 87, 113 and 117 were present in relative high concentrations in brioche, foccacia and the commercial bread BR9 (oat bran). Commercial bread BR5 (mixed grain), along the negative axis of PC 2, was found to have relatively high concentrations of masses m/z 33 and 45. PC3 distinguished ciabatta and foccacia

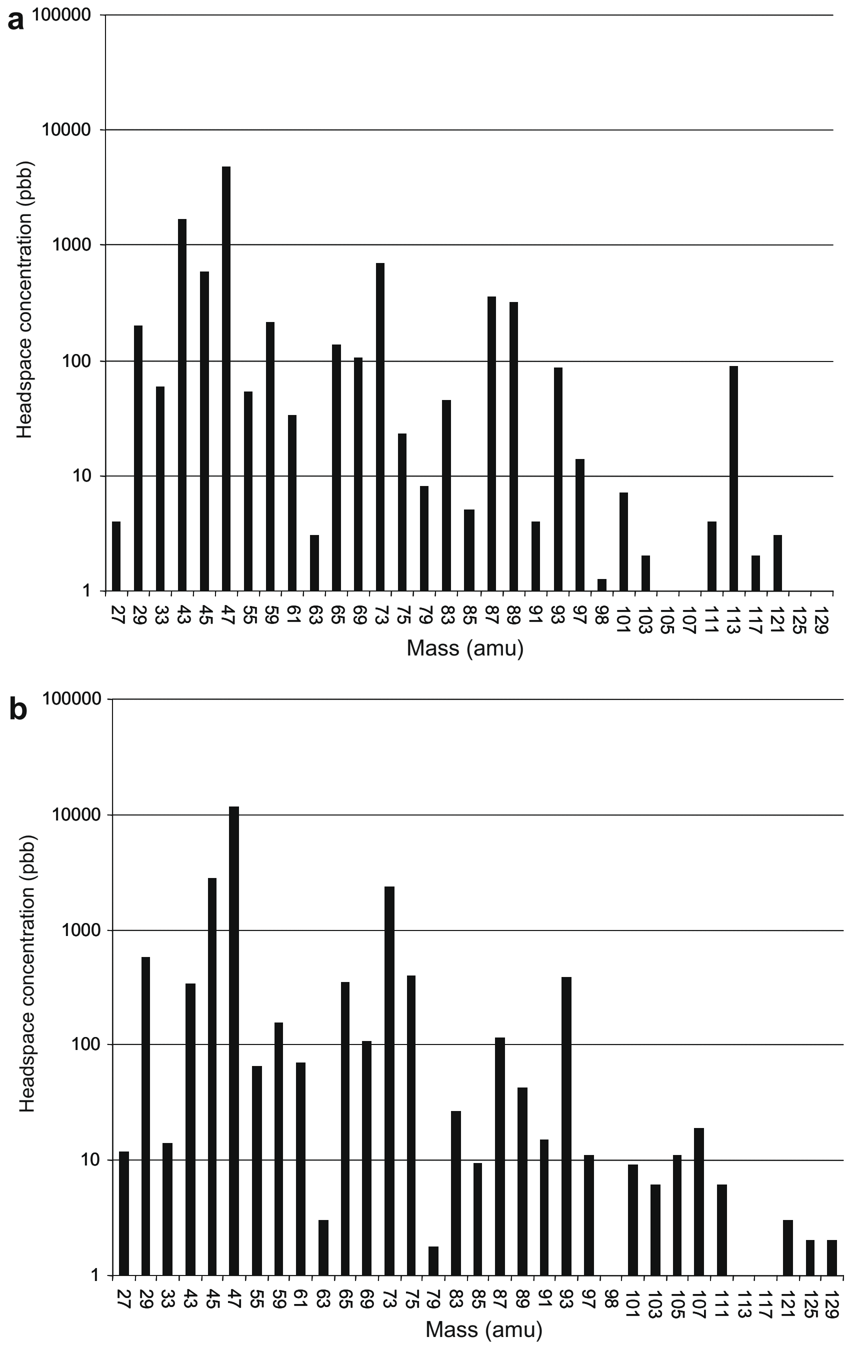

Fig. 2. Headspace spectra averaged over three repeated measurements of: (a) brioche, and (b) sourdough.

from rye bread, sourdough and pugliese bread, while PC4 separated rye bread, sourdough and commercial bread BR5 (mixed grain) from white bread and commercial breads BR4 (white) and BR8 (whole wheat) (Fig. 2b). Separation along PC3 was due to the relatively high concentrations of the mass ions m/z 117 and m/z 89 along the positive axis, and m/z 129. PC4 could be explained by mass ions m/z 101) and 113.

PCA of PTR-MS data, which accounted for 81% of the explained variance, discriminated samples just as well as the sensory data, where the first five PC's significantly ($p < 0.05$) discriminated between breads. This finding signifies the complexity of the differences between the volatile composition of breads and by doing so demonstrated the capability of the PTR-MS as a 'chemical finger printing' technique. This finding supports previous empirical evidence, where it was demonstrated that the latent structure in volatile composition of whey (Gallardo-Escamilla et al., 2005), cheese (Biasioli et al., 2006; Gasperi et al., 2001) and custard dessert (van Ruth et al., 2004) samples determined by PTR-MS analysis were similar to the latent structure in a trained panel's cognitive perception of the respective samples. Under these circumstances relationships between sensory and chemical data can be directly investigated.

3.3. PLS modelling and prediction of sensory character and bread freshness by volatile composition

Direct relationships between mass spectral finger prints and individual sensory attributes were investigated using a subset of 15 fresh breads. Subsequently, predictive power of each model could be tested using a validation set of five commercial breads

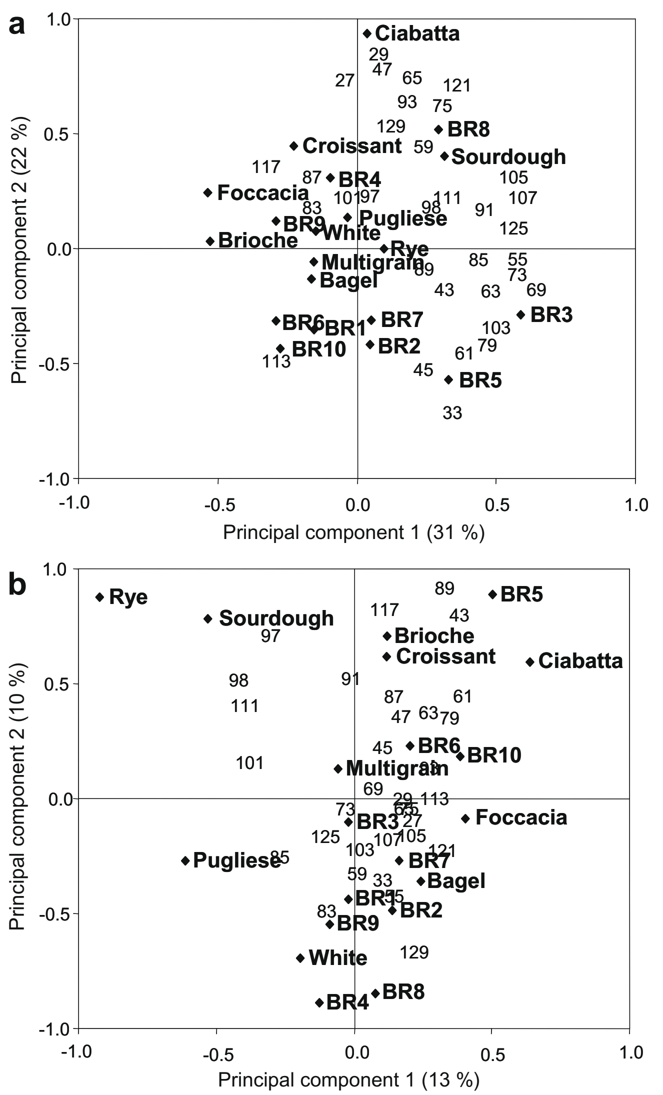

Fig. 3. Results of Principal Component Analysis biplot showing mass ion intensities of the specialty breads and commercial breads (BR1–BR10) for the first two components.

for which known measured sensory intensities could be compared. Visual inspection of PCA biplots revealed that the 15 bread types (ciabatta, sourdough, foccacia, brioche, rye, pugliese, white, bagel, croissant, multigrain and commercial breads BR3 (Swiss rye), BR5 (mixed grain), BR4 (white), BR10 (baguette) and BR8 (whole wheat)) spanned both the sensory and volatile distribution reasonably well. In accordance with Helgesen and Naes (1995), these samples accounted for the sensory and volatile distribution of the first five PCs, which explained 86% of the explained variance in the sensory data, and 81% of the explained variance in the PTR-MS data, respectively. In addition, a separate model that related volatile composition to consumer freshness perceptions of the 10 specialty breads was created.

Of the 18 sensory attributes measured, five odours, five flavours and one after-flavour were found to be correlated to a subset of mass ions (Table 2). Separately, consumer freshness perceptions of the breads were correlated with a subset of 12 mass ions. Successful regression models were recognised by calibration coefficients of $\geqslant$0.71, which expressed the strength of current models, whilst validation coefficients, which represented the models ability to predict new samples, were $\geqslant$0.63. Predictive performance was based on minimum error in the root mean square error of prediction (RMSEP) using full cross validation to select the optimum number of PLS factors for predicting the *Y*-data sets. For sensory attributes, the RMSEP values ranged from 4.70 to 9.13 (on the scale which measured sensory intensity between 1 and 100 mm). The RMSEP values obtained signified that all models had good predictive ability for the sensory attributes of the 15 bread types upon which models were built. Optimum model performance for "grain", "yeasty" odours, "sweet" flavour, and "sour" after-flavour were obtained using two PLS components, whilst the remaining sensory attributes were better modelled using three PLS components. However, for the sensory attributes of "floury", "nutty", "toasted" odours, "salty", "seedy" flavours and "bitter", "toasted" after-flavours, calibration, validation and RMSEP values (not shown) represented high variability, indicating poor model stability, or inability to identify any mass ions related to these sensory attributes. RMSEP for predictions of consumer freshness perceptions showed that the average uncertainty expected was 7.19, based on freshness intensity measured on a 150 mm scale, indicating good predictive power for freshness of the 10 specialty breads used in building the model. For freshness, optimum model performance was achieved using two PLS components.

Taken collectively, PLS results revealed that "dairy", "malty" odours, and "sweet", "buttery" flavours shared similar volatile profiles in terms of positively and negatively correlated masses *m/z* 87, 97, 117 and 63, respectively (Table 2). In comparison, the sensory attributes "grain", "musty" odours, and "sour" flavour shared positively correlated masses of *m/z* 63, 69 and 91. In addition, bread perceived to be most fresh shared a similar combination of positively correlated masses, *m/z* 87, 97 and 117, also represented by "dairy" odour and "buttery" flavour, whilst masses *m/z* 63, 69 and 91 that were negatively associated with bread freshness were represented by the sensory attributes "grain", "musty" odours, and

Table 2
Results of PLS1 regression between the mass ion signals (*X*-variables) and the sensory attributes (*Y*-variables) of the 15 selected bread types.

Sensory attribute	Positive correlations	Negative correlations	Calibration	Validation	RMSEP
O-Dairy	87, 97, 117	83, 91, 113, 121	0.96	0.88	7.13
O-Yeasty	29, 61, 79, 73	113, 33	0.71	0.65	5.26
O-Grain	63, 69, 85, 101, 107	27, 113	0.85	0.70	9.13
O-Musty	63,69,79,91,105	113	0.94	0.84	5.68
O-Malty	97, 98, 117	63, 113	0.83	0.79	8.71
F-Sweet	43, 97, 117	91, 121, 63	0.96	0.80	6.13
F-Sour	61, 63, 73, 85, 91, 105	27, 129	0.91	0.73	6.14
F-Bitter	45, 61, 75, 93, 111	59, 117, 129	0.89	0.63	3.29
F-Buttery	87, 93, 117	63, 91, 101, 111	0.93	0.81	5.31
F-Oily	79, 83, 101	63, 113	0.90	0.81	4.70
AF-Sour	61, 91, 93, 73	33, 59, 129	0.89	0.75	6.32
Freshness	55, 59, 87, 97, 117, 129	63, 69, 91, 93, 101, 121	0.95	0.73	7.19

RMSEP, root mean squares of prediction; *O*, odour, *F*, flavour, *AF*, after-flavour.

Table 3
Results of predictions showing predicted sensory characteristic intensity scores (Y-variables), reference (measured mean panel scores) for the twenty bread types.

Sensory attributes	Multigrain	Croissant	Bagel	Focaccia	white	Sourdough	Brioche	Pugliese	Ciabatta	Rye	BR3	BR4	BR5	BR8	BR10	r^a	BR1[c]	BR2[c]	BR6[c]	BR7[c]	BR9[c]	r^b
O-Dairy	7, 9	82, 84	16, 20	24, 31	11, 9	16, 18	84, 79	10, 9	14, 22	5, 6	8, 6	13, 13	11, 15	5, 6	16, 15	*0.92*	**15, 18**	**24, 10**	**37, 24**	**13, 13**	**7, 9**	0.72
O-Yeasty	35, 37	50, 44	35, 38	40, 44	36, 32	41, 36	24, 28	33, 29	42, 38	30, 40	40, 45	34, 26	40, 35	35, 39	27, 24	*0.68*	**38, 40**	**41, 30**	**42, 7**	**38, 34**	**26, 28**	-0.24
O-Grain	71, 66	1, 2	9, 8	2, 3	14, 12	14, 16	1, 3	6, 9	11, 12	28, 23	70, 98	10, 12	63, 74	67, 55	6, 4	*0.94*	**57, 48**	**4, 21**	**8, 2**	**64, 63**	**39, 17**	0.85
O-Musty	32, 36	9, 17	11, 24	21, 17	5, 12	17, 27	4, 18	11, 10	17, 15	11, 12	31, 31	11, 13	27, 27	29, 28	10, 7	*0.80*	**26, 24**	**19, 19**	**19, 16**	**37, 39**	**17, 15**	0.99
O-Malty	9, 12	4, 4	2, 1	1, 4	2, 1	4, 5	3, 6	2, 3	3, 7	86, 47	18, 12	1, 2	7, 9	2, 9	2, 8	*0.97*	**6, 7**	**1, 2**	**2, 1**	**11, 5**	**3, 11**	0.22
F-Sweet	7, 12	72, 71	18, 17	8, 12	12, 9	13, 19	56, 53	10, 13	13, 14	78, 70	17, 16	15, 13	24, 26	7, 11	8, 5	*0.97*	**20, 18**	**37, 1**	**45, 3**	**24, 22**	**7, 9**	-0.53
F-Sour	38, 31	25, 22	35, 34	42, 40	19, 19	37, 41	20, 23	22, 18	31, 33	19, 26	33, 32	13, 15	39, 42	30, 30	17, 19	*0.92*	**26, 19**	**19, 19**	**13, 19**	**21, 26**	**19, 18**	0.17
F-Bitter	11, 12	5, 4	8, 8	17, 12	5, 9	11, 13	5, 5	15, 11	16, 15	12, 11	18, 20	9, 9	17, 19	11, 11	10, 9	*0.88*	**10, 11**	**15, 15**	**5, 6**	**16, 13**	**8, 8**	0.95
F-Buttery	4, 5	83, 87	11, 12	26, 27	10, 14	14, 13	78, 76	14, 18	15, 13	7, 4	12, 16	13, 5	14, 24	4, 12	3, 8	*0.98*	**11, 12**	**17, 14**	**26, 22**	**4, 6**	**5, 8**	0.99
F-Oily	22, 20	16, 16	17, 20	77, 68	8, 6	23, 27	18, 16	15, 10	25, 23	7, 12	27, 28	13, 12	36, 36	16, 15	5, 5	*0.98*	**36, 29**	**15, 13**	**19, 15**	**24, 18**	**10, 15**	0.92
AF-Sour	23, 20	20, 22	24, 18	40, 21	15, 17	36, 28	18, 19	20, 17	28, 32	11, 12	25, 31	17, 18	35, 30	16, 22	10, 15	*0.70*	**20, 16**	**15, 16**	**20, 15**	**9, 8**	**10, 16**	0.56
Freshness	38, 40	68, 71	51, 51	69, 63	54, 57	37, 37	57, 59	56, 57	54, 50	65, 63	51	53	8	58	19	*0.96*	57	42	50	55	54	

O, odour, *F*, flavour, *AF*, after-flavour.
Intensity scores indicated in the table for each sensory attribute are; measured, predicted.
[a] Pearsons correlation between measured and predicted intensity are for samples used in buildings models.
[b] Pearsons correlation between measured and predicted intensity are for samples used for validation.
[c] The five breads excluded from models (validation set) predicted and measured sensory intensities are shown in bold; High deviation between predicted vs measured sensory intensities are shown for breads that are underlined.

"sour" flavour. Volatiles that were possibly responsible for mass ion signals could be tentatively assigned with reference to fragmentation patterns of pure compounds analysed by PTR-MS under standard conditions (Buhr, van Ruth, & Delahunty, 2002; Yeretzian, Jordan, & Lindinger, 2003). According to Buhr et al. (2002) mass ion m/z 87 may originate from diacetyl, 2-methylbutanal or 2-pentanone, while Yeretzian et al. (2003) reported that m/z 97 could possibly be assigned to furfural. Among these volatiles diacetyl was assumed to be responsible for the "buttery" odour associated with fresh bread flavour (Kirchhoff & Schieberle, 2001; Zehentbauer & Grosch, 1998b) and furfural has been previously described as having a brown, toasted flavour associated with bread (Chang et al., 1995; Seitz et al., 1998) However, lack of chromatographic separation of compounds limits the ability of PTR-MS as a species-specific quantitative method of analysis. In volatile mixtures, compounds and their fragments often share the same observed signal for a particular mass ion, which complicates the interpretation of PTR-MS spectra. It is important to note that without analysis of compounds as standards, PTR-MS did not definitively identify key chemical compounds found in different bread types. The aim of this study was to demonstrate the application of the data-driven technique for chemical finger printing as opposed to chemical identification.

According to Martinez-Anaya (1996), no single volatile compound can be considered the key component responsible for bread aroma. From this perspective, volatile constituents act in a synergistic way in relation to their relative proportions, which in turn can be modified by other substances that are present in breads (Richardmolard, Nago, & Drapron, 1979). Similarly, the present study demonstrated that individual odour and flavour attributes of bread depends on a mixture of specific volatiles. Subsequently, the application of this approach may facilitate a better understanding of the proportions and even absence of volatiles that elicit particular sensory characteristics, which in turn influence bread freshness. However, it is important to stress that correlations between individual sensory attributes and mass ion intensities, does not necessarily imply causality. Hence, models represented in this study should be interpreted as showing associations rather than direct cause and effect relationships. PLS1 in this study extracted the most relevant mass ions for predictive performance. Using a similar approach to determine relationships between PTR-MS fingerprints of volatile mixtures present in Trentingrana cheese and their sensory attributes, Biasioli et al. (2006) showed good modelling performance with PLS1.

Model predictions for sensory attribute intensities, alongside measured sensory intensities, are presented in Table 3. In addition, model predictions for consumer freshness perception intensities and measured freshness perception intensities are shown for the 10 specialty breads, while predicted freshness intensities are represented for the 10 commercial breads not evaluated by consumers. Pearson correlation coefficients are shown, which indicate the strength of the correlation between measured and predicted intensities. These have been calculated for samples used to build PLS models, and separately for samples not included in the building of models (validation).

Measured and predicted sensory intensity were very well correlated ($r > 0.88$) for samples that were used in the construction of models for all attributes apart from "yeasty" and "sour-after-flavour". On the other hand, the predictive ability of models for new samples (samples not included in built models) varied. Models for the attributes "dairy", "grain" and "musty" odour, "bitter", "buttery" and "oily" flavour had good predictive ability ($r > 0.72$). However other attribute models did not perform as well and those for "yeasty" odour and "sweet" flavour had very poor predictive ability. This result could be explained by the robustness of models and the type of breads used for validation. Commercial bread BR6 (panini) deviated the most from measured to predicted sensory intensity. In this case, BR6 will have been somewhat of an outlier in terms of the relationship between its volatile composition and sensory character, due to the presence or absence of compounds that can influence the overall perception of the mixture.

Measured and predicted freshness were very well correlated ($r = 0.96$) for the 10 specialty breads that were used in building the perceived freshness model. In this case, freshness was not measured for the commercial breads BR1-BR10, and so the predictive ability of the model could not be externally validated. Commercial sample BR5 (mixed grain), and to some extent BR10 (baguette), showed considerably low levels of predicted freshness intensities when compared with the other commercial breads. In this instance it is important to note that consumer freshness perceptions for these breads may have been influenced by sensory sensations other than odour and flavour. Previous work that related sensory attributes to consumer freshness perceptions demonstrated that "porous" appearance positively influenced freshness, whilst "adhesive" texture was negatively associated with bread freshness (Heenan et al., 2008).

Overall, these results demonstrated that the volatile information used to build the current models had direct relevance on the sensory attributes perceived by the trained panel. Furthermore, volatile profiling by PTR-MS demonstrated promising opportunities in determining bread freshness that may be used as a rapid technique to predict whether newly developed bread products will be perceived by consumers as fresh at the time of sale.

4. Conclusion

The research clearly showed that volatile information acquired by PTR-MS analysis can be applied to model and characterise the sensory properties of different bread types. In addition, PTR-MS can be used to predict consumers' perceptions of the freshness of different bread varieties that are all equally fresh in terms of elapsed time from baking. PTR-MS analysis and sensory evaluation enabled the selection of 15 breads that ensured a good representation of both the sensory and volatile composition of bread types and allowed predictive models to be built. Sensory attribute prediction model validation using a subset of five samples provided a robust measure of each models predictive power. Clearly, the results of this study showed promising opportunities for rapid profiling and screening of bread sensory quality and with a view towards the perceived freshness of bread.

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