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Multivariate statistical analysis for the identification of potential seafood spoilage indicators

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ABSTRACT

Volatile organic compounds (VOCs) characterize the spoilage of seafood packaged under modified atmospheres (MAs) and could thus be used for quality monitoring. However, the VOC profile typically contains numerous multicollinear compounds and depends on the product and storage conditions. Identification of potential spoilage indicators thus calls for multivariate statistics. The aim of the present study was to define suitable statistical methods for this purpose (exploratory analysis) and to consequently characterize the spoilage of brown shrimp (*Crangon crangon*) and Atlantic cod (*Gadus morhua*) stored under different conditions (selective analysis). Hierarchical cluster analysis (HCA), principal components analysis (PCA) and partial least squares regression analysis (PLS) were applied as exploratory techniques (brown shrimp, 4 °C, 50%CO_2/50%N_2) and PLS was further selected for spoilage marker identification. Evolution of acetic acid, 2,3-butanediol, isobutyl alcohol, 3-methyl-1-butanol, dimethyl sulfide, ethyl acetate and trimethylamine was frequently in correspondence with changes in the microbiological quality or sensory rejection. Analysis of these VOCs could thus enhance the detection of seafood spoilage and the development of intelligent packaging technologies.

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1. Introduction

Modified atmosphere packaging (MAP) is commonly used for perishable food products such as seafood in order to inhibit or delay microbial growth and thus to extend the shelf life and quality of the packaged product. During microbiological spoilage of foodstuffs, decomposition of available nutrients by microbial activity can lead to the generation of volatile organic compounds (VOCs) associated with both primary and secondary metabolism (Wang, Li, Yang, Ruan, & Sun, 2016). Growth of specific spoilage organisms (SSOs) and subsequent production of off-odors into the package headspace eventually causes consumer rejection (Gram & Dalgaard, 2002). Consequently, odor is considered as one of the most important seafood quality parameters (Olafsdottir, Jonsdottir, Lauzon, Luten, & Kristbergsson, 2005; Olafsdóttir et al., 1997).

Microbial spoilage of fish may manifest itself as sweet, fruity, ammonia-like, putrid and sulfuric off-odors. VOCs contributing to the odor of fish can be divided into three groups, specifying compounds associated with freshness (C_6-C_9 alcohols and carbonyl compounds), lipid oxidation (aldehydes) and microbiological spoilage (Olafsdóttir et al., 1997). According to Olafsdóttir et al. (1997), microbiological spoilage odor is generally due to compounds such as ammonia, ethanol, ethyl acetate, hydrogen sulfide, 3-methyl-1-butanol, methyl mercaptan and trimethylamine. However, the composition and the development of the VOC profile are affected by several factors, including food product, headspace gas composition, temperature, initial contaminating microbiota and microbial metabolism (Wang et al., 2016).

Brown shrimp (*Crangon crangon*) is highly susceptible to

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microbiological spoilage. Shrimp contains high amounts of free amino acids and other readily available nutrients for microbial growth (Zeng, Thorarinsdottir, & Olafsdottir, 2005). Unlike other crustaceans, shrimp cannot be kept alive for extended periods before processing (Adams & Moss, 2008). Currently, the shelf life of preservative-free cooked brown shrimp is maximally 4–6 days under refrigerated conditions (Broekaert, Heyndrickx, Herman, Devlieghere, & Vlaemynck, 2013).

Since microbial activity is the main cause of fish spoilage (Gram & Dalgaard, 2002), identification and quantification of VOCs produced during microbial metabolism under different packaging and storage conditions could enhance efficient quality analysis of the packaged product. Evolution of these spoilage indicators in relation to microbial growth and sensory rejection could be used for the development of intelligent packaging applications. Generally, concentrations of VOCs that indicate spoilage can be expected to increase as a function of storage time and progressing microbial growth. However, VOCs are produced and degraded as a result of several biological and chemical processes. Furthermore, certain odors may be considered as a part of natural odor in one foodstuff and rejected in another product (Gram & Dalgaard, 2002). Thus, the complexity of concentration evolution and acceptancy as well as the wide number of potential spoilage indicators calls for multivariate statistical analysis.

Different statistical methods have been applied to multivariate microbiological and chemical data, including hierarchical cluster analysis (HCA), principal components analysis (PCA) and partial least squares regression analysis (PLS). Previously, PCA has been applied to the comparison of different food products (Blixt & Borch, 2002), microbiota (Hierro et al., 2005; Verginer, Leitner, & Berg, 2010), treatments (Ciesa et al., 2013) or times of storage (Duflos et al., 2010; Fik, Surówka, Maciejaszek, Macura, & Michalczyk, 2012). PLS has been used for the analysis of progressing microbial growth on the basis of VOC concentrations (Jørgensen, Huss, & Dalgaard, 2001; Marín et al., 2007; Storer, Hibbard-Melles, Davis, & Scotter, 2011) and also applied along with HCA or PCA (Argyri, Doulgeraki, Blana, Panagou, & Nychas, 2011; Argyri, Mallouchos, Panagou, & Nychas, 2015; Blixt & Borch, 2002; Mataragas, Skandamis, Nychas, & Drosinos, 2007; Mikš-Krajnik, Yoon, Ukuku, & Yuk, 2016; Siroli et al., 2014; Vervoort et al., 2012; Wibowo, Grauwet, Gedefa, Hendrickx, & Van Loey, 2015).

The aims of the present study were to 1) determine suitable multivariate statistical methods for characterizing the VOC profile of seafood (exploratory analysis) and 2) consequently identify the most potential spoilage indicators of Atlantic cod (*Gadus morhua*) and brown shrimp stored under different modified atmosphere (MA) conditions (selective analysis). Firstly, HCA, PCA and PLS were applied as exploratory techniques to microbiological, chemical and/or sensory data. Comparison of the three techniques was carried out using a dataset collected during refrigerated storage of seafood (brown shrimp, 4 °C, 50%CO_2/50%N_2) where selected-ion flow-tube mass spectrometry (SIFT-MS) was used for the quantification of VOCs from the package headspace. On the basis of the exploratory analysis, PLS was chosen to be used in selective analysis. Independent PLS analyses were carried out for data collected during spoilage of Atlantic cod (Kuuliala et al. submitted manuscript) and brown shrimp under different packaging and storage conditions.

2. Materials and methods

2.1. Data collection

The datasets used in the study were collected during individual storage experiments of brown shrimp (2×) or Atlantic cod (5×) and used for exploratory (brown shrimp, 4 °C, 50%CO_2/50%N_2) or selective (all storage experiments) statistical analyses.

2.1.1. Brown shrimp

The two individual storage experiments of brown shrimp consisted of sample preparation and packaging, real-time quantification of VOCs with SIFT-MS, microbiological analysis and sensory evaluation.

2.1.1.1. Raw material. Brown shrimp were caught in the North Atlantic Ocean (FAO zone 27) in October and November 2015. The shrimp were sorted according to size and washed before cooking according to normal Belgian fishing practices. No additives or preservatives such as benzoic or sorbic acid were added during processing. After cooking, the shrimp were cooled and stored overnight in plastic bags under ice. The shrimp were brought onshore the following morning and directly transported to the Laboratory of Food Microbiology and Food Preservation (LFMFP, UGent) where the batch was hand peeled. During peeling, shrimp were kept on ice in plastic bags while avoiding direct contact between shrimp and ice. Shrimp portions of 150 ± 2 g were packaged at 2:1 headspace-product ratio with a tray sealer (MECA 900, DecaTechnic, Herentals, Belgium) using multilayer packaging trays (PP/EVOH/PP, oxygen transmission rate 0.03 cm^3/tray*24 h at 23 °C and 50% R.H.) and top film (PA/EVOH/PA/PP, oxygen transmission rate 6.57 cm^3/m^2*24 h*atm at 23 °C, 50% R.H. and 1 atm). Two individual batches of shrimp were independently packaged under modified atmospheres ($CO_2/O_2/N_2$%) 50/0/50 or 30/0/70 and stored at (4.0 ± 0.7) °C prior to analyses. Analyses were carried out on days 0 (day of packaging), 3, 5, 7, 10 and 12 for three randomly chosen packages (A-C). New replicates A-C were analyzed on each day of storage due to the destructive nature of the microbiological analyses. After sampling, the remaining shrimp was packaged under vacuum using high barrier film bags (oxygen transmission rate < 2.7 cm^3/m^2*24 h*bar at 23 °C and 0% R.H.) and stored at −32 °C for no longer than 70 days.

2.1.1.2. Quantification of spoilage related VOCs by SIFT-MS. The principles of selected-ion flow-tube mass spectrometry have been described in previous studies (Noseda et al., 2010). VOCs (Table 1) were selected on the basis of previous research and literature and quantified from the package headspace by a spectrometer (Voice 200, Syft Technologies™, Christchurch, New Zealand). Package headspace was sampled through a septum inserted on the package lid with a flow rate of 25.6 ml/min for 60 s (preparation 10 s, sample 50 s) and the concentrations were averaged over eleven data points. A certain package was sampled twice. During sampling, the headspace was connected to atmospheric air with a needle inlet in order to avoid collapse and changes in the internal conditions of the package.

The relative standard deviation ($SD_{\%}$) of each VOC concentration during an individual SIFT-MS scan was calculated as follows:

$$SD_{\%} = SD_m/x_m*100\% \quad (1)$$

where x_m is the average and SD_m the standard deviation of a single SIFT-MS scan (n = 11). VOCs with concentrations exceeding 25% average $SD_{\%}$ during the entire storage time within a certain packaging condition were considered not to allow sufficiently accurate quantification and were thus excluded from further analyses.

2.1.1.3. Microbiological analysis. Each shrimp sample of 30 ± 0.1 g was aseptically weighed into a sterile stomacher bag, diluted ten times in physiological saline peptone solution (PPS; 0.85% NaCl, 0.1% peptone) and homogenized in Stomacher Lab Blender (LED

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