Food Quality and Preference 19 (2008) 609–617

Contents lists available at ScienceDirect

Food Quality and Preference

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

Prediction of sensory quality in raw carrots (*Daucus carota* L.) using multi-block LS-ParPLS

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ARTICLE INFO

Article history:
Received 25 April 2007
Received in revised form 4 March 2008
Accepted 31 March 2008
Available online 18 April 2008

Keywords:
Daucus carota
Sensory profiling
Multi-block analysis
Principal component analysis (PCA)
LS-ParPLSc

ABSTRACT

The relations between the sensory quality of 24 different carrot genotypes and content of dry matter, non-volatile and volatile compounds were studied using a multi-block approach called LS-parPLS. The prediction of five sensory attributes; bitterness, sweetness, terpene flavour, green flavour and carrot flavour, gave prediction errors (RMSECV) between 0.98 and 1.36 and correlation coefficients (r) between 0.60 and 0.81. The explained Y-variances were between 15.1% and 66.0%. The highest prediction error was observed for the attribute carrot flavour whereas green flavour gave the best prediction. The attributes green flavour, bitterness and terpene flavour showed fairly good predictions (r/RMSECV/% exp-Y = 0.81/0.98/66.0, 0.79/1.23/62.3 and 0.71/1.04/50.2) whereas sweetness gave an unexpected poor prediction (r/RMSECV/% exp-Y = 0.67/1.36/44.6). Non-volatile compounds found to be important predictors were chlorogenic acid (5-CQA), sucrose, 6-methoxymellein (6-MM), falcarindiol (FaDOH), and falcarinol (FaOH). The volatile compounds found to be important predictors are considered as key flavour compounds of raw carrots: terpinolene, β-pinene, sabinene, γ-terpinene, α-pinene, β-bisabolene, caryophyllene and cuparene. In general, the overall results show that the sensory quality variation in the material regarding bitterness, green flavour and terpene flavour are explained by relatively few parameters. Despite that the results revealed some reliable relationships between the sensory attributes, aroma and chemical analysis, a large variance (about 40%) in the sensory block of variables remained unexplained and still needs further investigation for an in-depth understanding of sensory quality. LS-ParPLSc is shown to be feasible for handling several types of data blocks in one regression model.

1. Introduction

Horticulturists have been working on genetic approaches for improving nutrient content and visual appeal of vegetables in hopes of increasing consumer consumption of beneficial phytochemicals. Consumers have shown an increased interest in healthy food and an increased demand for diversity in vegetables (Jongen, 2000) and in order to be able to act on changing consumer demands, it is important to have quantitative means for assessing quality and quality changes in vegetables. Biological materials such as carrots are complex substances that usually have uncontrollable variations in quality. These variations can arise from genetics, environmental conditions or be due to pre-processing (Baardseth et al., 1996; Hogstad, Risvik, & Steinsholt, 1997; Rosenfeld, Aaby, & Lea, 2002; Seljåsen, Bengtsson, Hoftun, & Vogt, 2001a; Simon, Peterson, & Lindsay, 1980). Carrot genotypes with different colours (orange, red, yellow, purple and white) are now available on the market and they show a large diversity in quality (Alasalvar, Grigor, Zhang, Quantick, & Shahidi, 2001; Kreutzmann, Christensen, & Edelenbos, 2008; Kreutzmann, Thybo, & Bredie, 2006).

Carrots have a number of chemical and physical quality characteristics and the eating quality can be probed directly by sensory methods or indirectly by chemical, mechanical, or optical measurements. Important properties are contents of sugars, dry matter, non-volatile bitter compounds and volatile compounds. However, it is a challenge to understand exactly which chemical compounds and combination of compounds that affect the sensory-perceived quality.

Multivariate data analysis using ordinary principal component analysis (PCA) and partial least squares (PLS) regression are well known when trying to understand the sensory quality in relation to physical and chemical properties of carrots (Kreutzmann et al., 2008; Kreutzmann, Thybo, Christensen, & Edelenbos, in press; Rosenfeld et al., 2002; Seljåsen et al., 2001a). Trying to identify which chemical analysis and individual components that are having high impact on the sensory attributes can be overwhelming even with general PCA and PLS regression. Multi-block (MB) analysis is one approach capable of handling data where several types of analysis or blocks structures are present. Several approaches for

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doi:10.1016/j.foodqual.2008.03.007

performing MB analysis have been suggested and compared through out the years. Wangen and Kowalski (1988) suggested a MBPLS algorithm based on the MBPLS algorithm from Wold, Martens, and Wold (1984). Wold, Kettaneh, and Tjessam (1996) published an approach referred to as hierarchical MBPLS. The hierarchical MBPLS and the MBPLS are similar in the way they combine the common information in a super level described by super scores and super loadings. Westerhuis, Kourti, and MacGregor (1998) showed that MBPLS provides the same predictions as an ordinary PLS under the condition that the weighting and scaling are the same. Furthermore they suggested another approach where deflation is to be performed on the super scores instead of the block scores of the X blocks as Wangen and Kowalski originally suggested. Westerhuis and Smilde (2001) altered the deflation step of the method suggested by Westerhuis et al. (1998) using only the super scores to deflate the Y response and not change the X blocks. An alternative MB approach is the serial-PLS (S-PLS) suggested by Berglund and Wold (1999). This method shows resemblance to the iterative least squares PLS (LS–PLS) purposed by Jørgensen, Segtnan, Thyholt, and Næs (2004), Jørgensen, Mekvik, and Næs (2007). Måge (2006) followed up on the LS–PLS and suggested the LS-parallel-PLS (LS-parPLS) and LS-parPLS with common components (LS-parPLSc). These methods will be described in detail later in the data analysis section.

One of the main problems with most MB methods have been how to determine the proper block scaling. Depending on how the data blocks are scaled, very different results, hence interpretations can be obtained. The LS-parPLS and LS-parPLSc methods both avoid the block scaling effect as they are invariant to scaling and are capable of handling different complexities of the individual block contributions. Måge (2006) compared the most frequently used MB methods based on two case studies with design variables and parallel blocks of spectroscopic measurements. The predictive performance and interpretability were compared. The study concludes that the models performed equally well in their predictive performance if properly used whereas differences were be found in the ability to provide meaningful interpretation of the models. When the information in the X blocks was overlapping the LS-parPLSc model reflected the true data structure in the best way whereas situations with no overlapping information was best modelled by the LS-parPLS. The present study will focus on the LS-parPLSc method. Originally, this method was suggested when modelling designed data where information in addition to a design can be split up into intuitively meaningful blocks (e.g. volatile and non-volatile compounds) (Mekvik, Jørgensen, Måge, & Næs, submitted for publication). The information in the dependent variables related to the design matrix is extracted from additional blocks before modelling the influence of these. If the experiment is not designed the design step can be eliminated and the remaining blocks are then analysed in such a way that any common structure between the blocks is analysed separately from unique information. LS-parPLSc provides an excellent visualizing and data interpretation tool, as scores and loadings for each data block contribution are given. This is where the LS-parPLSc distinguishes itself from the ordinary PLS regression as it calculates a regression model based on all data material but keep the structure of individual block contributions. An ordinary PLS regression has to be performed either on one single block at a time or if many blocks are present they have to be combined in on big block.

The aim of the present work was to investigate which chemical compounds or combinations of compounds are important for the sensory quality of raw carrots. In order to predict the sensory quality from the raw material measurements the non-volatile compounds, contents of sugars, dry matter (Block I) are combined with the volatile compounds (Block II) in one regression model using LS-parPLSc. The main goal is to find a good model that explains the variation in the end product well and to interpret the given model parameters in order to obtain information about which variables are important and in what way they seem to affect the sensory quality.

2. Materials and methods

2.1. Plant material and sample preparation

Twenty-four different carrot genotypes were selected to represent a large variation in odour and taste by sensory screening of 50 genotypes. The genotypes were grown in Denmark, Norway and Holland during 2004 and harvested at the end of October 2004. The carrots obtained from Denmark were cultivated at Research Centre Aarslev, those from Norway were cultivated at Plante Forsk, The Norwegian Crop Research Institute, Hedmark and those obtained from Holland were cultivated by Bejo Zaden B.V., Warmenhuizen. The roots were transported to Research Centre Aarslev and stored at 1 °C until February 2005 at >95% relative humidity (RH). All roots were stored in an ethylene free atmosphere except for Bolero. A sample of this cultivar was moved to apple storage facilities and exposed to ethylene generated by the apples one month before sensory evaluation (Kidmose et al., 2004; Seljåsen, Hoftun, & Bengtsson, 2001b). The root weight varied from approximately 50–150 g. However, the most representative size within each genotype was selected for analysis. Samples (8 kg) of carrots were taken from each genotype and divided into sub-samples of 1.5–2.0 kg carrots of first class quality, i.e. carrots with no visible damage representing each replicate. The carrots were then carefully washed, manually hand-peeled and trimmed. Approximately 0.65–1.00 mm of the periderm was removed by peeling and 2 cm of the tip and 2 cm of the top was also removed by trimming. The peeled carrots were cut into $2 \times 2 \times 20$ mm sticks using a food processor (Robot Coupe CL50, Vincennes Cedex, France), carefully mixed and samples of 1500 g were taken for immediately analysis of sensory quality, volatile compounds and phenolic acids. All analysis was carried out in three replicates. The rest of the raw carrots were frozen at −24 °C until analyzed for polyacetylenes, isocoumarin, sugars and dry matter content 2–4 months later.

2.2. Sensory analysis

Quantitative descriptive analysis was performed as previously described (Kreutzmann et al., 2008). A panel consisting of 10 trained assessors (5 females/5 males, aged from 26 to 54 years) evaluated the sensory quality in terms of 4 odour attributes, 7 flavour attributes, 2 taste attributes, and 1 aftertaste attribute. The fourteen attributes were: terpene aroma, carrot aroma, green aroma, faded aroma, terpene flavour, carrot flavour, green flavour, faded flavour, nutty flavour, soapiness, sickenly sweet flavour, bitterness, sweetness and burning aftertaste. The sensory laboratory and the computer screens were illuminated with red light during evaluation to mask visual differences between samples. The panellists evaluated the samples at individual speed by descriptive analysis on an unstructured 15 cm line scale with intensity ratings ranging from low (value 0) to high intensity (value 15). All data was registered on a direct computerised registration system (FIZZ, ver. 2.00 M, Couternon, F).

2.3. Chemical analysis

Extraction and quantification of the polyacetylenes falcarindiol (FaDOH), falcarindiol 3-acetate (FaDOAc), falcarinol (FaOH) and 6-methoxymellein (6-MM) were performed by solvent extraction and reversed phase-high performance liquid chromatographic