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Sensors and Actuators B 116 (2006) 107–115
SENSORS AND ACTUATORS B CHEMICAL
www.elsevier.com/locate/snb

The electronic tongue and ATR–FTIR for rapid detection of sugars and acids in tomatoes

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Received 10 July 2005; received in revised form 29 September 2005; accepted 30 November 2005
Available online 27 April 2006

Abstract

The electronic tongue and attenuated total reflectance–Fourier transform infrared spectroscopy (ATR–FTIR) have been evaluated as novel rapid techniques in taste research. The electronic tongue, consisting of 27 potentiometric sensors, and ATR–FTIR, a well-established spectroscopic technique, have been used to determine the sugar and acid profile of four tomato cultivars: Aranca, Climaks, Clotilde and DRW 73-29. The most abundant sugars (glucose, fructose and sucrose) and organic acids (citric acid, malic acid, tartaric acid, fumaric acid and succinic acid) in tomatoes were measured with HPLC as a traditional reference technique. The ability of the novel techniques to detect differences in sugar and acid profiles between these four tomato cultivars has been studied by means of unsupervised and supervised multivariate data analysis techniques such as principal components analysis (PCA) and canonical discriminant analysis (CDA). Canonical correlation analysis (CCA) was applied to compare the information content of the reference technique with that of the electronic tongue and ATR–FTIR. The potential of both the electronic tongue and ATR–FTIR to predict the chemical composition of a sample has been evaluated using partial least squares (PLS) models. Both the electronic tongue and ATR–FTIR have the potential to measure taste determining compounds. Tomato cultivars can be classified based on their sugar and acid profile. However, the prediction of individual components in tomato juice is still inaccurate and needs further optimization.

Keywords: Tomato; Acids; Sugars; HPLC; Electronic tongue; ATR–FTIR; Multivariate data analysis

1. Introduction

Traditionally, sensory and instrumental techniques are used to determine the taste of horticultural commodities. In sensory analysis taste is evaluated by trained panels or consumer panels. Although sensory panel analysis is by far the most realistic technique to obtain information on human taste and aroma perception, it has some problems including the correctness of training, standardization of measurements, stability and reproducibility. Two other drawbacks of this technique are the high cost and taste saturation of the panelist [1].

Instrumental analytical techniques such as high pressure liquid chromatography (HPLC), gas chromatography (GC), soluble solids content (Brix %), titratable acidity (TA) and pH give information on the chemical composition of the sample and, hence, are useful to describe the taste profile of the product. These traditional techniques however often require a laborious and time-consuming sample preparation. Other drawbacks are the high cost and the need for skilled people to operate the equipment [2].

Recently some new paths have been explored to develop an alternative for the traditional techniques. Different multisensor systems, called electronic tongues, have been developed over the last decade [3]. The basic idea behind electronic tongue technology is the application of an array of non-specific chemical sensors with a high cross-sensitivity, i.e. a wide selectivity towards several components. Discrimination and classification, quality evaluation and control, process monitoring and quan-

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doi:10.1016/j.snb.2005.11.084

titative analysis of foodstuff and beverages have successfully been performed with electronic tongues. The main advantages of electronic tongues are the low cost, easy-to-handle measurement set-up and speed of the measurements [4]. Several research groups focus on electronic tongue development. A first type of electronic tongue has been developed by Toko in Japan. The taste sensor is composed of eight potentiometric sensors with lipid/polymer membranes. The measured potential of this system is converted into measures for taste quality and intensity. It works through the principle of global selectivity which implies the ability to classify chemical substances into groups, as found in biological taste reception. The electronic tongue developed by Toko has been applied in qualitative discrimination of mineral waters, beverages and foodstuffs [5,6]. A second type of electronic tongue was developed by Winquist et al. at the Swedish Sensor Centre, S-SENCE. The voltammetric electronic tongue has been applied for the classification of beverages and environmental monitoring of drinking water [7]. A hybrid electronic tongue based on a combination of voltammetric metallic electrodes and potentiometric ion-selective electrodes has been developed and applied for the classification of fermented milk [8]. A third type of electronic tongue, which will be used in this paper, was developed at the Saint-Petersburg University in Russia. The electronic tongue is based on specially designed non-specific, weakly selective potentiometric chemical sensors with an enhanced cross-sensitivity to as many components in solution as possible [3,9]. These non-specific sensors are comprised into sensor arrays producing multidimensional response, which contains information on several components or groups of components in a complex sample [2,3]. The electronic tongue is capable of both qualitative recognition and quantitative determination of taste. It has been applied in the research for polluted waters [10], quantitative analysis of mineral water and wine [11], analysis of beverages [12], recognition of liquid and flesh food [13], analysis of Korean green tea [4] and the evaluation of Italian wine [2].

Another alternative for traditional instrumental techniques is Fourier transform infrared spectroscopy (FTIR), a well-established technique in chemical analysis. Through FTIR spectrometry with advanced optics and a high signal-to-noise ratio, detection of individual components as well as subtle compositional differences between and among complex samples is possible [14]. Mid infrared has been less employed than the near infrared due to the high absorbance of aqueous solutions, which drastically affects the sensitivity. FTIR has been used to predict sugar contents in both agricultural and food products [15,16]. In addition, attenuated total reflectance (ATR–FTIR) measurements offer interesting possibilities for the analysis of samples containing solids and liquids. ATR–FTIR successfully resulted in the determination of sucrose in beetroot [17], organic acids and sugars in apple juices [18] and caffeine in soft drinks [19]. In the last few years there has been a shift towards flow injection FTIR analysis. This technique reported successful for the determination of sucrose and glucose [20,21] and the discrimination of red wines, edible oils and beer [22–24].

The objective of this study is to evaluate the potential of the electronic tongue and ATR–FTIR as fast techniques to classify new and commercially available tomato cultivars according to their sugar and acid profile. Hereto, first, the information content of the electronic tongue and ATR–FTIR will be compared to that of the HPLC reference technique. Second, the ability of the electronic tongue and ATR–FTIR to predict the chemical composition of the tomatoes will be investigated using multivariate statistical techniques.

2. Materials and methods

2.1. Plant material

Four tomato cultivars (*Lycopersicon esculentum* Mill.) were selected for this experiment: Aranca, Climaks, Clotilde and DRW 73-29. Twenty tomatoes per cultivar were harvested at the Proefstation voor de Groenteteelt in Sint-Katelijne-Waver (Belgium) at ripeness stage 6 (breaker class) [25]. The tomatoes were stored for 1 day at ambient atmosphere, 18 °C and 80% relative humidity. The day after harvesting the tomatoes were cut in pieces and frozen in liquid nitrogen. The frozen samples were stored at −80 °C until further sample preparation was performed.

2.2. HPLC

The frozen tomato samples were ground into a fine powder. The grinding was partly performed by hand, using a mortar, and partly mechanically with a homogenizer (MM 200, Retsch, Haan, Germany). The powder, 0.1 g, was transferred into a cooled 1.5 ml eppendorf tube (Eppendorf, Hamburg, Germany) and again stored at −80 °C until the extraction of the samples was performed. The organic acids and sugars were extracted by adding 500 μl of 80% (v/v) ethanol to the frozen samples. After incubation in a temperature controlled shaker (Thermomixer Comfort, Eppendorf, Hamburg, Germany) at 78 °C and 850 rpm during 10 min, and centrifugation at 4 °C and 14,000 rpm during 5 min (Hawk 15/05 Refrigerated centrifuge, Sanyo, Bensenville, USA) the supernatants was transferred in two new eppendorf tubes. For the analysis of organic acids 300 μl of supernatants was used, for sugars 100 μl. Subsequently the eppendorfs were dry centrifuged (Concentrator 5301, Eppendorf, Hamburg, Germany). For organic acid and sugar analysis, respectively, 100 and 200 μl of HPLC water (Fisher Scientific, Loughborough, UK) was added to the samples. After incubation, at the same conditions as mentioned before, the samples were filtered on a 0.45 μm pore space filter (Alltech Associates Inc., Deerfield, USA).

The analysis of the organic acids and sugars were carried out on a Series 1100 HPLC (Agilent, Palo Alto, USA). The acids were separated on a Prevail Organic Acid column (Alltech Associates Inc., Deerfield, USA) at room temperature with a mobile phase of formic acid (pH 2.5). The organic acids were detected with a diode array detector (DAD) at 200 nm. The sugars were separated on an Aminex column (Bio-Rad, Hercules, USA) with water as mobile phase and at a column temperature of 80 °C. The sugars were detected with a refractive index detector (RID). Chemstation software Version 10.01 (Agilent, Palo