Analytica Chimica Acta 634 (2009) 172–179

Contents lists available at ScienceDirect

Analytica Chimica Acta

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

Prediction of sensory properties of Brazilian Arabica roasted coffees by headspace solid phase microextraction-gas chromatography and partial least squares

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ARTICLE INFO

Article history:
Received 23 September 2008
Received in revised form 11 December 2008
Accepted 12 December 2008
Available online 25 December 2008

Keywords:
Processed coffee
Solid phase microextraction
Correlation optimized warping
Principal component analysis and partial least squares

ABSTRACT

Volatile compounds in fifty-eight Arabica roasted coffee samples from Brazil were analyzed by SPME-GC-FID and SPME-GC-MS, and the results were compared with those from sensory evaluation. The main purpose was to investigate the relationships between the volatile compounds from roasted coffees and certain sensory attributes, including body, flavor, cleanliness and overall quality. Calibration models for each sensory attribute based on chromatographic profiles were developed by using partial least squares (PLS) regression. Discrimination of samples with different overall qualities was done by using partial least squares-discriminant analysis (PLS-DA). The alignment of chromatograms was performed by the correlation optimized warping (COW) algorithm. Selection of peaks for each regression model was performed by applying the ordered predictors selection (OPS) algorithm in order to take into account only significant compounds. The results provided by the calibration models are promising and demonstrate the feasibility of using this methodology in on-line or routine applications to predict the sensory quality of unknown Brazilian Arabica coffee samples.

According to the PLS-DA on chromatographic profiles of different quality samples, compounds 3-methypropanal, 2-methylfuran, furfural, furfuryl formate, 5-methyl-2-furancarboxyaldehyde, 4-ethylguaiacol, 3-methylthiophene, 2-furanmethanol acetate, 2-ethyl-3,6-dimethylpyrazine, 1-(2-furanyl)-2-butanone and three others not identified compounds can be considered as possible markers for the coffee beverage overall quality.

1. Introduction

The establishment of mechanisms that allow the evaluation, assurance and certification of the quality of food products is an indispensable strategy for maintaining commercial competitiveness. The great number of norms created by international organizations, like the International Organization for Standardization (ISO), indicates the importance of the quality guarantee determined by a set of parameters, frequently used in commercial transactions [1]. These measurable parameters must be faced as an essential element to improve the aggregate value of the agro-industrial production worldwide. To attain an objective guarantee, research has been carried out for better evaluation of the coffee beverage in order to correlate its quality with physicochemical characteristics and the chemical composition of green or roasted beans [2–7].

Commonly, the quality of coffee is evaluated according to criteria such as bean size, color, shape, cupping and number of defects [2,6,8,9]. However, cupping, also known as cup tasting, is still the most widespread technique employed to evaluate the final quality of this product. Arabica coffee, generally regarded as superior to Robusta coffee in terms of sensory attributes, accounts for approximately 70% of world production of this commodity [10].

Flavor plays an important role in sensory analyses and could be considered a "fingerprint" of products, but despite its importance, there are few studies that correlate this characteristic with the final quality of coffee beverage [9]. This correlation, using multivariate analysis [11], is an excellent tool in the quality control of foods and agricultural products and is being applied successfully in analyses of hazelnut, vinegar, juices and wine [12–16].

The chemistry of coffee flavor is highly complex and is still not completely understood. The main families of chemical compounds

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doi:10.1016/j.aca.2008.12.028

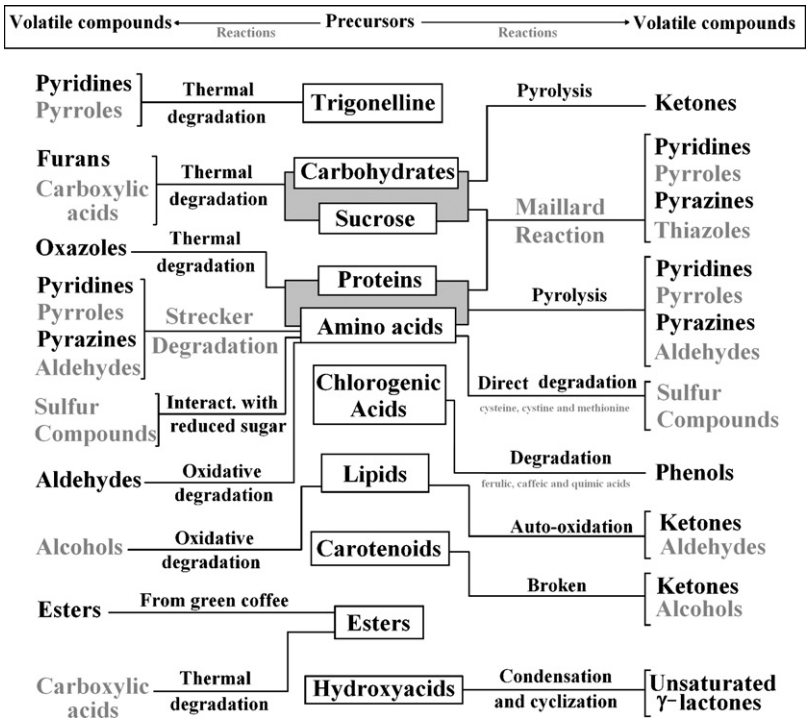

Fig. 1. Schematic representation of the main volatile formation reactions during the coffee roasting process.

found in green coffee, and responsible for the volatiles in roasted coffee, are alkaloids like trigonelline, chlorogenic acids, carbohydrates, free sugars like sucrose, lipids and proteins. During the roasting process, the composition of coffee beans is drastically changed and several hundreds of substances associated with coffee flavor and taste are formed [17]. A general description of the volatile compounds, their precursors and the main volatile formation reactions are shown in Fig. 1.

Several efforts have been made to identify the main volatile compounds responsible for the real flavor of roasted coffee [18–25]. However, the question of which volatiles are the most relevant contributors for the quality of coffee has not yet been elucidated.

Among the analytical techniques used to analyze and separate volatile fractions of different products, gas chromatography has been established as one of the most important. Coupled with gas chromatography, solid phase microextraction (SPME) has been shown to be an excellent sampling method, allowing simultaneous extraction and concentration of analytes from sample matrices [26].

With the aim to identify characteristic volatile compounds that could be responsible for prediction of certain sensory attributes of Brazilian Arabica coffee, chromatographic profiles and sensory profiling were compared in this work using chemometric data treatment.

2. Materials and methods

2.1. Coffee samples

Fifty-eight Arabica green (not roasted) coffee samples from different origins were supplied by Instituto Agronômico de Campinas. Flat coffee beans were visually inspected, and those with defects like black, insect-damaged, immature and broken were excluded. The roasting process was carried out in a gas faired drum roaster (Pinhalense S/A Máquinas Agrícolas) to the medium roast point. Roasted coffee samples were packed in films consisting of plastic (polystyrene and polyethylene) and aluminum, to avoid aroma losses and contamination by external substances, and stored at −5 °C for a maximum period of 48 h before chromatographic analyses.

2.2. Sensory analysis of the coffees

All 58 Arabica coffee samples were evaluated by two cuppers. The cup quality was assessed by flavor, body, cleanliness and overall quality using sample preparation according to Brazilian legislation (Normative instruction no. 8, from 11 June 2003) obtained from www.pr.gov.br/claspar/pdf/cafebenef008_03.pdf.

Thus, for the four sensory attributes selected for evaluation a fivepoint scale was adopted, in such a way that each of the attributes, according to the degree of sensory magnitude perceived were given corresponding scale points, e.g., the cleanliness classifications 'rio' (1) and 'strictly soft' (5) defined the extreme scores on the rating scale.

2.3. SPME devices and GC-FID parameters

SPME fibers coated with 65-μm thick polydimethylsiloxane/divinylbenzene (PDMS/DBV) and the manual holder were purchased from Supelco (Bellefonte, PA). The fibers were conditioned according to the SPME data Sheet (T7941231) from Supelco in the GC injector port. The analyses were performed on a G-6850 GC-FID system (Agilent, Wilmington, DE) fitted with a HP-5 capillary column (30 m × 0.25 mm × 0.25 μm). Helium (1 mL min^{-1}) was the carrier gas. The oven temperature was programmed as follows: 40 °C → 5 °C min^{-1} → 150 °C → 30 °C min^{-1} → 260 °C. The injection port was equipped with a 0.75 mm i.d. liner and the injector was maintained at 220 °C in the splitless mode. Under these conditions, no sample carry-over was observed on blank runs conducted between extractions.

Identification of the extracted analytes was performed on a HP-5890 gas chromatographer (Hewlett-Packard, Wilmington, DE, USA) equipped with a HP-5973 mass-selective detector fitted with the same column and operated under the same conditions as