Food Chemistry 145 (2014) 802–806

Contents lists available at ScienceDirect

Food Chemistry

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

Chilean flour and wheat grain: Tracing their origin using near infrared spectroscopy and chemometrics

Ma Inmaculada González-Martín [a], Guillermo Wells Moncada [b], Claudio González-Pérez [a], Nelson Zapata San Martín [b], Fernando López-González [a], Iris Lobos Ortega [a], Jose-Miguel Hernández-Hierro [a,*]

[a] Departamento de Química Analítica, Nutrición y Bromatología, Facultad de Ciencias Químicas, C/Plaza de la Merced s/n., 37008 Salamanca, Spain
[b] Facultad de Agronomía Universidad de Concepción, Av. Vicente Méndez 595, Chillán, Chile

ARTICLE INFO

Article history:
Received 23 March 2013
Received in revised form 25 August 2013
Accepted 27 August 2013
Available online 6 September 2013

Keywords:
Near-infrared spectroscopy
Geographical origin
Wheat
Flour
Chemometrics

ABSTRACT

Instrumental techniques such a near-infrared spectroscopy (NIRS) are used in industry to monitor and establish product composition and quality. As occurs with other food industries, the Chilean flour industry needs simple, rapid techniques to objectively assess the origin of different products, which is often related to their quality. In this sense, NIRS has been used in combination with chemometric methods to predict the geographic origin of wheat grain and flour samples produced in different regions of Chile. Here, the spectral data obtained with NIRS were analysed using a supervised pattern recognition method, Discriminat Partial Least Squares (DPLS). The method correctly classified 76% of the wheat grain samples and between 90% and 96% of the flour samples according to their geographic origin. The results show that NIRS, together with chemometric methods, provides a rapid tool for the classification of wheat grain and flour samples according to their geographic origin.

1. Introduction

The importance of the control of food authenticity is increasing due to expanding global markets. The relative ease, with which food products can be transported between the different zones of a country, and even between continents, means that consumers are becoming progressively more concerned about the origin of the products they consume.

In the case of wheat grain and its derivatives (flours), different methods have been used to achieve such aims. The vegetation is the compositional reflection of the bio-available and mobilized nutrients presents in the underlying soils on which they are cultivated. Cereal quality can be impacted by a number of factors during the production process such as seeding date, varieties, planting practices. Moreover, other factors such as nutrient, weed, disease, insect and irrigation managements also present a great impact on cereal quality (Kansas-State-University, 1997). Element availability depends on several factors, such as soil, pH, humidity, porosity, clay and humic complexes etc. (Kim & Thornton, 1993). Consequently, the range of soils presents in a given area and bioavailability provide markers in foods that characterise their geographical origin (Gonzalez, Gallego, Valcarcel, & Gomez-Cardenas, 2001). The analysis of certain stable isotopes has also proved to be a robust tool that can be used to determine the geographic origin of many food products. The usual method is to take advantage of the isotopic ratios of hydrogen ($^{2}H/^{1}H$) and of oxygen ($^{18}O/^{16}O$), although those of carbon ($^{13}C/^{12}C$) and nitrogen ($^{15}N/^{14}N$) are also used (Kelly, Heaton, & Hoogewerff, 2005). The natural isotopic abundance ratios of carbon, oxygen and nitrogen were determined and a comparison was made between the isotopic contents of durum wheat semolina samples originating from Italy and those of samples originating from other countries (Australia, Canada, Turkey) (Brescia et al., 2002a; Brescia et al., 2002b), and a correlation was found between the isotopic composition and geographic origin of the samples. In an additional study in which the authors employed the spectroscopic technique known as proton high-resolution magic angle spinning nuclear magnetic resonance (^{1}H HR-MAS NMR), two cultivars of durum wheat produced in different Italian geographical areas were differentiated according to cultivar and geographical origin using multivariate statistics (Brescia et al., 2002a; Brescia et al., 2002b). A preliminary investigation was carried out (Branch, Burke, Evans, Fairman, & Wolff Briche, 2003) to examine the utility of ICP-MS elemental isotope analysis of Cd, Pb, Se and Sr plus stable isotope gas analysis of ^{13}C and ^{15}N with multivariate statistics in identifying the country of origin of *Triticum aestivum* L. It was found that the samples could be classified geographically using a simple analyte, $\delta^{13}C$, and that

* Corresponding author. Current address: Food Colour & Quality Lab., Dept. of Nutrition & Food Science, Universidad de Sevilla, Facultad de Farmacia, 41012 Sevilla, Spain. Tel./fax: +34 923294483.
E-mail address: jmhhierro@usal.es (J.-M. Hernández-Hierro).

0308-8146/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.foodchem.2013.08.103

the methodology showed some potential in identifying different cultivars and blends within a region using discriminant analysis.

The genetic diversity of high- and low-molecular weight glutenin subunits of 63 landrace durum wheat samples from different geographical regions in the Mediterranean Basin was studied using SDS–PAGE. Considerable variability in the gluten in composition was found. The relationship between different regions of origin has been discussed (Moragues, Zarco-Hernandez, Moralejo, & Royo, 2006).

Recently, (Teklu, Hammer, & Röder, 2007) investigated the genetic diversity of 73 different types of wheat from 11 geographic zones, correlating the results with the zone of production by multivariate principal component analysis. (Brandolini, Hidalgo, & Moscaritolo, 2008) determined the magnitude of different parameters (texture, proteins, ashes, etc.) in the Einkom variety of wheat (*Triticum monococcum* L Subsp. *trionococcum*) from different geographic areas, observing different mean values in nearly all the parameters as a function of the zone of origin.

In Chile, about 300 thousand hectares of wheat are harvested every year and almost 88% come from the Maule Region (VII Region), Bio Bio (VIII Region) and La Araucanía (IX Region). These regions are located from latitude 34°51'S to 39°30'S, covering some 500 km from North to South, thus being subject to highly, varied geography and climatology (Fig. 1). The Wheat Flour Regulation Nch 1237-2000 (Instituto-Nacional-de-Normalización, 2000) looks for quality attributes oriented towards final use, the uniformity of requirements and certification by region, because the zone of wheat production can be used to characterize the composition and foreseeable yield of the raw materials.

With a view to discriminating among three different production zones in Chile (Regions VII, VIII and IX), in the present work NIRS technology was employed together with Discriminat Partial Least Squares (DPLS), allowing decisions to be made regarding the traceability of the Chilean wheat grain and flour samples in a simple, rapid and precise way that does not require sample destruction.

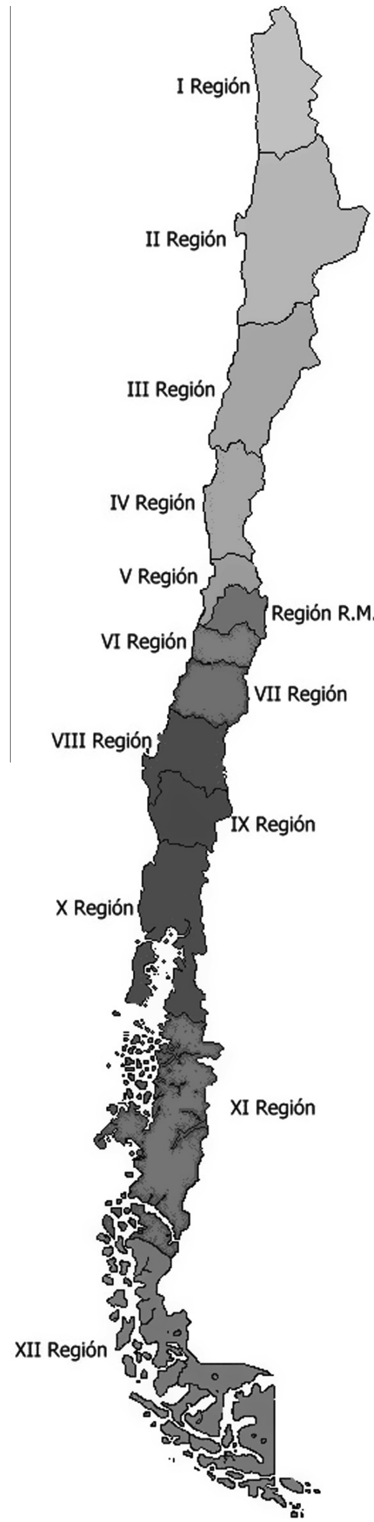

Fig. 1. Chilean regions to which the samples studied correspond.

2. Materials and methods

2.1. Wheat grain and flour samples

The wheat grain samples (249) were collected from three geographic zones of Chile (Regions VII, VIII and IX) and their corresponding flours were also used. The samples come from the mills and cooperatives in each of the regions under study, and have been carefully chosen to ensure representativeness of the wheat production in Chile. The total number of samples collected by Region, sowing seasons, and wheat varieties are shown in Table 1. The table highlights the differences in the sowing season of the different regions studied, which points to considerable variability as well as showing the number of different varieties used in each case.

2.2. Edaphoclimatic characteristics of the study area

The three geographic regions of Chile (VII, VIII and IX) where wheat samples were collected have clear differences in soil and climate. The VII Region (11.8% of Chilean wheat) has a temperate climate with 4–5 dry season months (November to March), with annual rainfall reaching 750 mm, which are concentrated in winter (from June to August). The average annual temperatures of this Region vary between 13 and 15 °C. In Region VII, wheat production occurs in the Andean foothills on Inceptisols soils. In the coastal area on soils derived from granite rocks which are highly eroded and with low productive capacity. In the central valley of Region VII wheat crops are grown on Vertisols and Alfisols, very clayey and good fertility. Region VIII (30.2% of Chilean wheat) has a temperate climate with dry season similar to the VII region, but at lower temperatures due to increasing latitude. The average annual temperature is below 13 °C. Rainfall exceeds 1000 mm per year, which are concentrated in winter. Wheat production in this region is mainly carried out on Inceptisols soils, which are located in the foothills of the Andes, these soils have developed from volcanic ash, have low pH and high phosphorus retention. In the Central