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Prediction of wheat tortilla quality using multivariate modeling of kernel, flour, and dough properties☆

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ABSTRACT

Traditional wheat quality methods for bread have poor predictive power for flatbread quality, which impedes genetic improvement of wheat for the growing market. We used a multivariate discriminant analysis to predict tortilla quality using a set of 16 variables derived from kernel properties, flour composition, and dough rheological properties of 187 experimental hard wheat samples grown across Texas. A discriminant rule (suitability for tortillas = diameter > 165 mm + day 16 flexibility score > 3.0) was used to classify samples. Multivariate normal distribution of the data was established (Shapiro–Wilk $p > 0.05$). Logistic regression and stepwise variable selection identified an optimum model comprising kernel weight, glutenin–gliadin ratio, insoluble polymeric proteins, and dough extensibility and stress relaxation parameters, as the most important variables. Cross-validation indicated 83% model prediction efficiency. This work provides important insight on potential targets for wheat quality genetic improvement for tortillas and specialty product market.

Industrial relevance: Tortillas and other flatbread manufacturers currently use wheat developed for other commodities and rely on trial and error, and use of various additives to optimize product quality. Genetic development of wheat for these markets is impeded by lack of knowledge of specific grain quality parameters to target. With the growing demand for clean label and healthy offerings by consumers, the industry is looking for natural ingredients with improved functionality. This work provides the first insight into the specific wheat composition and functional parameters that can predict tortilla quality.

1. Introduction

Tortillas and other specialty breads are increasingly becoming a global dietary staple. For example, according to the Tortilla Industry Association report for 2013, wheat tortilla was the only bakery segment that experienced growth in 2012 and is projected to increase further (TIA, 2013). Wheat tortilla sales exceeded $6 billion in 2012, affirming consumer preference for its versatility and functional convenience. To consumers, the definition of good quality tortilla encompasses its ability to retain flexibility and be large enough to wrap food (Waniska et al., 2004).

Despite the growing popularity of tortillas, the main challenge is that there is no reliable and practical method to predict wheat (*Triticum aestivum* L.) functionality for tortillas, as is the case with pan bread and other mainstream baked products. Currently, most tortilla ingredient suppliers and processors use trial and error and additives to optimize tortilla quality, which compromise sensory appeal and quality, and add to cost of manufacture. The health conscious consumer is also increasingly demanding use of fewer additives (clean label), as well as healthier options, like whole grains. Thus there is a need to develop wheats with improved functionality for the tortilla and flatbread market. However, effective genetic improvement efforts require that the key grain quality parameters responsible for desirable product characteristics can be reliably identified. Ideally the methods to identify these grain quality factors should be rapid and require a small sample size. Currently, the only way to predict wheat functionality for tortillas is to actually make the product.

Tortilla quality in the USA is largely defined by diameter, flexibility during storage, and opacity (Alviola & Awika, 2010; Alviola, Jondiko, & Awika, 2010). Earlier studies reported that tortillas of good quality can be produced using wheat flour of intermediate protein content, protein strength and low level of starch damage (Waniska et al., 2004). However, the vast majority of wheat that fall in this category did not produce a good quality product (Waniska et al., 2004). Tortilla diameter can be predicted using linear equations comprising mixing time and dough resistance to extension (Barros et al., 2010). However, these linear models did not significantly predict tortilla flexibility, which is a critical tortilla

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quality attribute. A major challenge to predicting tortilla quality is the negative correlation that generally exists between the main quality factors, tortilla diameter, and flexibility during storage (Mondal et al., 2008; Pascut, Kelekci, & Waniska, 2004). Large diameter generally requires weak and extensible dough, which tends to be detrimental to tortilla flexibility.

Genetic improvement of wheat targeting alterations of high molecular weight glutenin subunit (HMW-GS) composition through deletion at one or more of the *Glu A1*, *B1*, and *D1* loci has shown promise as a way to produce unique gluten functionality ideal for tortillas and other specialty products (Jondiko et al., 2012; Mondal et al., 2008; Tuncil et al., 2016; Zhang et al., 2014). There is a need to develop prediction models that can be used to screen these wheat varieties under development for end use functionality. Hence, this study used multivariate statistical methods designed to elicit information from simultaneous measurements of many variables acquired from wheat kernel, flour, and dough to predict the quality of tortilla, specifically the diameter and flexibility during storage. In addition, the study investigated whether these multivariate models could be used to reliably classify early to late generation wheat lines for their potential to produce good quality tortillas. The objectives of this study were to develop a model that can be used to predict the functional performance of wheat varieties for tortilla processing, and provide insight on wheat quality parameters that can be targeted for genetic improvement for specialty flatbread market.

2. Materials and methods

2.1. Experimental materials

A total of 187 hard winter wheat (HWW) lines were used. These included advanced generation breeding lines comprising 38 Texas elite (TXE) lines, 3 uniform variety trial (UVT) lines; 101 experimental lines derived from 'TAM111'/'TAM112' population (TAM1112); and 45 identity preserved lines specifically developed for specialty flatbreads (TIA). These TIA lines were selected based on variations in their allelic composition at the HMW-GS loci *Glu A1*, *Glu B1* and *Glu D1*. The wheat samples were grown in Texas A&M AgriLife experimental plots across Texas in 2009–2012 seasons.

2.2. Kernel properties and milling

The wheat lines were evaluated for hardness, diameter, weight and moisture content using a single kernel hardness tester (SKCS) (Perten Instruments, Springfield, IL, USA). The grains were tempered to 14% moisture content (AACC Method 26-50.01) and milled using a Quadrumat Senior mill (Brabender Instruments, South Hackensack, NJ, USA). Flour milling yields were recorded. The samples were processed into tortillas with 1–2 months after milling.

2.3. Evaluation of flour properties

2.3.1. Total protein content

Total flour protein content was determined in two replicates for each wheat line using near-infrared reflectance spectroscopy (Perten PDA 7000 Dual Array with Grams Software) according to AACC Method 39-11.01 (AACC-International, 2010).

2.3.2. Polymeric to monomeric protein ratio (glutenin to gliadin ratio)

The protein extraction of proteins followed the method of Gupta, Khan, & Macritchie (1993). Briefly, a 10 mg flour sample was mixed with 1 mL 0.05 M sodium phosphate buffer, pH 6.9, containing 0.5% SDS (*w*/*v*) then sonicated for 35 s at power setting 10 W. The sample was then centrifuged at 15,000×*g* for 5 min and the supernatant collected (contains total protein) and filtered through 0.45 μm filter and analyzed by size — exclusion HPLC using an Agilent 1260 HPLC (Agilent, Santa Clara, CA, USA), 300 × 7.8 mm BioSep-SEC-S400 column (Phenomenex, Torrance, CA, USA) with a gradient system composed of 50% ACN + 0.1% TFA (B) and 50% water + 0.1% TFA (A), 30 °C column temperature, at a flow rate of 1 ml/min for 30 min run. The chromatograms were manually integrated. The area of the first peak corresponds to total polymeric proteins and the area of the second peak to monomeric proteins (Gupta, Khan, & Macritchie, 1993). Two replicates of each flour sample were analyzed.

2.3.3. Insoluble polymeric protein content (IPP)

Ten milligrams of flour was suspended in 1 mL of 0.05 M sodium phosphate buffer (pH 6.9), containing 0.5% sodium dodecyl sulfate (SDS) and shaken on a vortex for 30 min. The mixture was then centrifuged for 5 min at 16,000×*g*. The supernatant (containing soluble polymeric protein — SPP) was collected and filtered (0.45 μm) and analyzed by size — exclusion HPLC as described above (Bean et al., 1998). The pellet was mixed with 1 ml sodium phosphate buffer and sonicated for 25 s at 10 W. The mixture was centrifuged at 16,000×*g*/5 min, and the supernatant collected and filtered as above then analyzed using the SE-HPLC as described above. The percentages of soluble (extractable) and insoluble (unextractable) polymeric protein were calculated as [peak 1 area (extractable)/peak 1 area (total)] × 100 and [peak 1 area (unextractable)/peak 1 area (total)] × 100 respectively. Peak 1 (total) refers to the sum of peak 1 (extractable) and peak 1 (unextractable).

2.3.4. High molecular weight to low molecular weight glutenin subunit ratio (H_L_GS_Ratio)

HMW-GS and LMW-GS were quantified using RP-HPLC. A sample of 100 mg flour was mixed with 1 mL sodium iodate buffer (0.3 M sodium iodate + 7.5% isopropanol) and vortexed for 15 min. The mixture was centrifuged for 5 min at 15,000×*g*. The supernatant containing gliadins was discarded. To the pellet 1 ml water was added then shaken for 5 min and centrifuged at 15,000×*g* for 5 min. The pellet was mixed with 1 mL 50% isopropanol containing 2% BME and vortexed for 30 min, and then centrifuged for 5 min. at 15,000×*g*. The supernatant was collected (contains glutenins) and 600 μL of the glutenin extract was alkylated with 40 μL 4-vinylpyridine for 15 min at 60 °C. The resulting sample was injected into a Phenomenex Jupiter C18 250 × 4.6 mm diameter column, 5 μ particle size, and 300 Å pore size. The solvent flow rate was 1.0 mL/min and composed of water (A) and acetonitrile (B), both containing 0.1% TFA. The gradient was as follows: 0–3 min from 25% B to 35% B, 3–24 min increased to 53%B, the gradient decreased to 25% B at 25 min and kept at 25% B until 29 min. Detection of protein peaks was carried out by UV detector at 210 nm. The area of the curve corresponding to HMW-GS and LMW-GS contents was determined by manual integration and the HMW/LMW-GS ratio was calculated (Cinco-Moroyoqui & MacRitchie, 2008; Fu & Kovacs, 1999; Suchy, Lukow, & Fu, 2003).

2.4. Dough mixing and rheology

2.4.1. Dough development time

A mixograph (National Manufacturing Co., Lincoln, NE, USA) was used to estimate dough mixing/development time and flour water absorption; 10 g of flour was used (14% mb) (AACCI Method 54-40.02; AACCI 2010). Mixing/dough development time was manually calculated from the mixograph by drawing two midlines from each end of the graph. The point of crossover was marked as the peak time for each wheat line (Alviola & Awika, 2010).

2.4.2. Dough compression force

Dough compression test was used to measure the maximum compression force required to deform a 45 g dough ball. Two dough balls were compressed to 70% of their height using a 10 cm diameter probe on a TA-XT2 texture analyzer (Texture Technologies Corp., Scarsdale,