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GlutoPeak profile analysis for wheat classification: skipping the refinement process

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KEYWORDS

GlutoPeak test; farinographic stability; whole grain flour; Principal Component Analysis; k-Nearest Neighbours classification

ABBREVIATIONS

AgrEn, Aggregation Energy; EnMT, Energy to Maximum Torque; EnPM, Energy after Maximum Torque; FS, farinographic stability; GPU, GlutoPeak Unit; MT, Maximum Torque; PCA, Principal Component Analysis; PMT, Peak Maximum Time.

ABSTRACT

The GlutoPeak test can predict wheat flour quality by measuring gluten aggregation properties in a short time and using a small amount of sample; thus has usefulness along the entire wheat delivery chain. However, no information on the suitability of this new test on whole grain flours is available. In this contest a multivariate approach was used to assess the GlutoPeak test ability to predict dough quality directly from whole grain flour. GlutoPeak test was performed on both refined and whole grain flours (22 samples), obtaining both profiles and calculated indices, which were subjected to data exploration through Principal Component Analysis. Results suggested a trend according to farinographic stability values. Furthermore, k-Nearest Neighbours classification models were developed using the GlutoPeak profiles to predict farinographic stability, leading to average prediction ability of 81.8% for both refined and whole grain flour data. The present outcome suggests the possibility of predicting farinographic stability by GlutoPeak test directly on whole grain flour, thus skipping the refinement process.

1. INTRODUCTION

Common wheat (*Triticum aestivum L.*) is the most suitable raw material for the production of a large number of products, including bread, biscuits, cakes, and noodles. The functionality and versatility of this cereal is associated with the capacity of its storage proteins - gliadins and glutenins - to form a gluten network that exhibits viscoelastic properties. However, although each wheat flour can organize its storage proteins into a viscoelastic network, different classes of wheat are suited for different types of products to deliver certain functional attributes. Indeed, hard wheat varieties are preferred for bread or others leavened products, where a strong gluten network is required; whereas soft wheat is preferred for cookies and cakes, where a weak gluten network is desirable. Even in the same class of wheat (e.g. hard wheat), not all the varieties perform the same during processing. In this regard, many rheological tests have been proposed - and successfully used - to predict wheat flour behaviour during dough mixing (e.g Farinograph, Mixograph, Mixolab), extension (e.g. Extensograph, Alveograph), leavening (e.g. Rheofermentometer) and baking (e.g. Mixolab) (Pagani, Marti, & Bottega, 2014). Most of these rheological approaches have to adapt with the changes and, thus, the new needs of the value chain of wheat, where: (i) breeders look for reliable methods to test the functional quality of wheat lines at early stages, with just a limited amount of sample, (ii) millers need fast and reliable methods for checking wheat quality at the receiving station, and (iii) the baking industry looks for suitable methods that could predict end product quality for production and product development (Marti, Augst, Cox & Koehler, 2015). In other words, the value chain of wheat is looking for a reliable test for the prediction of gluten functionality in a short time and using a small amount of sample. In this frame, the GlutoPeak test has been recently proposed for the evaluation of wheat flour quality based on gluten aggregation kinetics (Kaur Chandi & Seetharaman, 2012). Recent work has shown GlutoPeak potential for predicting gluten quality for noodle (Lu & Seetharaman, 2014) and pasta (Marti, Cecchini, D'Egidio, Dreisoerner, & Pagani, 2014) production. Moreover, the GlutoPeak indices have been used for predicting the conventional parameters related to dough mixing stability, extensibility, and tenacity (Marti, Ulrici, Foca, Quaglia, & Pagani, 2015).

Even if rheological analyses have a multivariate nature, few studies dealing with grain and cereal products treat the data with a chemometric approach (i.e. Pastor, Ačanski, Vujić, Bekavac, Milovac, & Kravić, 2016; Banu & Aprodu, 2015; Vidya, Ravi, & Bhattacharya, 2013). At present, Chemometrics is being more and more applied all along the food chain for general exploratory data analysis (through Principal Component Analysis - PCA) (Giovenzana, Beghi, Malegori, Civelli, & Guidetti, 2013), multivariate regression (such as Partial Least Square Regression - PLSR) (Malegori, Marques, de Freitas, Pimentel, Pasquini, & Casiraghi, 2017) and classification (with discriminant or one-class methods) (Oliveri & Downey 2012). In a previous study, Marti, Ulrici, Foca, Quaglia, & Pagani (2015) applied PCA and PLSR to investigate the correlations existing between the conventional wheat rheological parameters and the GlutoPeak indices. However, the mentioned approach relied on the GlutoPeak indices calculation from a dedicated software, whereas the direct extrapolation of relevant information from the GlutoPeak profile would reduce the calculation time, overcome the software dependence and capture its multivariate nature.

To the best of our knowledge, the GlutoPeak test has been applied only on refined flours, with the exception of the work done by Kaur-Chandi & Seetharaman (2012) with the aim of optimizing the method. Thus, the potential use of the GlutoPeak test on whole grain flours has not been explored yet, in view of describing wheat quality. Defining gluten quality directly on the wheat kernels would be of great interest for both breeders and millers, since it would predict wheat quality while skipping the refinement process, and thus saving time.

Taking into consideration the multivariate nature of rheological data, the aim of this study was to investigate GlutoPeak profiles by chemometric techniques for gluten aggregation properties prediction of both whole grain and refined flours. To the aim, a GlutoPeak data exploration step was performed through PCA, followed by the development of classification models for farinographic stability prediction by k-Nearest Neighbours algorithm (Vandeginste, Massart, Buydens, De Jong, Lewi, & Smeyers-Verbeke, 1998). Moreover, the possibility of using the GlutoPeak curve of whole grain flours for the assessment of the refined wheat flour quality category was also investigated, following the same approach proposed for refined wheat flour. This study would provide information whether it would be possible to predict dough properties from whole grain samples without the need for the refining process, thus allowing the classification of a sample according to end-product functional attributes immediately at raw material acceptance.

2. MATERIALS AND METHODS

2.1 Materials

A set of 22 hard red spring wheat varieties were cultivated in 2011 in Crookston (MN, US). Whole grain flours were obtained by grinding the seeds with a Cyclone Sample Mill (UDY Corp., Fort Collins, CO) equipped with a 0.25 mm screen. From the same source samples, refined flours were obtained by conditioning (to 15.5 g/100g moisture overnight) and milling the seeds with a Quadrumat Junior (C.W. Brabender Inc., South Hackensack, NJ, USA).

2.2 Farinograph Test

Grain samples were analyzed for mixing properties using the Farinograph-E (CW Brabender Instruments, Inc., South Hackensack, NJ, US) equipped with a 10 g mixing bowl (AACCI 54–21, 2000).

2.3 GlutoPeak Test

Gluten aggregation properties were measured using the GlutoPeak device (C.W. Brabender Inc., South Hackensack, NJ, USA), as reported by Kaur-Chandi & Seetharaman (2012). An aliquot of 8.5 g of sample (refined and whole grain flour) was dispersed in 9.5 g of 0.5 mol L^{-1} $CaCl_2$, scaling both solvent and flour weight on a 14% flour moisture basis in order to keep the liquid-to-solid ratio constant. Sample temperature was maintained at 34 °C by circulating water through the jacketed sample cup. The paddle was set to rotate at 1900 rpm and the test was carried out for 7 min.

2.4 Data processing

2.4.1 Index calculation

The main indices automatically evaluated by the software provided with the GlutoPeak device (Brabender GlutoPeak v. 2.1.2) are: *i)* the Peak Maximum Time (PMT, expressed in s), corresponding to the time before torque falling off when gluten breaks down; *ii)* the Maximum Torque (MT, expressed in GlutoPeak Unit - GPU), corresponding to the peak occurring due to gluten aggregation; *iii)* aggregation energy (AgrEn, expressed in GlutoPeak Unit - GPU), corresponding to the area under the curve between 15 s before and 15 s after MT. In addition, the following indices were calculated using Microsoft Excel 2010 (Microsoft, Redmond, VA): *iv)* Energy to Maximum Torque (EnMT; expressed in arbitrary units - AU) corresponding to the area of the curve from the beginning of the test and MT; *v)* Energy after Maximum Torque (EnPM; expressed in arbitrary units - AU) corresponding to the area of the curve from the beginning of the test and 15 s after MT.

2.4.2 Multivariate approach

The GlutoPeak profiles collected from the 22 wheat flour samples, as well as a dataset composed by the calculated indices, were submitted to two separated PCA after data mean centering. The same approach was followed for the data collected by analysing the related whole grain flours. Beyond being a powerful tool for data visualization (Jolliffe, 1986), PCA provided an understanding of the relationships between all the variables (i.e. variables which contribute similar information to the model) and among variables and samples. Thus, it was possible to compare samples patterns in each PCA model obtained with both GlutoPeak profile and calculated indices; in addition, the variables' weight in the new defined plane was assessed.

As a first attempt, linear classification methods (namely, linear discriminant analysis – LDA – on the principal component scores, and partial least square discriminant analysis – PLS-DA) were applied, but these techniques did not provide satisfactory results in terms of classification rate (data not shown). This indicated a non-linear method to be required. The K-nearest neighbors (K-NN) technique was chosen for the classification of both whole grain and refined flour, being one of the less prone to overfitting thanks to the simplicity of its algorithm, which does not include optimization of numerous parameters. The definition of the two "a priori" classes was based on the FS value, allowing to obtain two balanced classes in term of number of constituents. K-NN, without making any assumptions on the underlying data distribution, keeps all the training data (the 22 GlutoPeak profiles) and calculates the Euclidean distance of the data points in their metric space. In our case, using the 1-nearest neighbour classifier, the simpler nearest neighbour type classifier, the algorithm assigns each sample to the class of its closest neighbour in the feature space (Dudoit, Fridly, & Speed, 2002). The reliability of the classifier was tested by leave-one-out cross-validation due to the reduced dimension of the dataset. The error rate of each k-Nearest Neighbour classifier was expressed as prediction rate. Data processing was carried out by a Matlab R2016a (The MathWorks. Inc, USA) routine.

3. RESULTS AND DISCUSSION

3.1 Mixing properties and gluten aggregation kinetics

Table 1 reports the farinographic stability (FS) values of refined flours from hard red spring wheats. All the analysed flour samples exhibited a mixing profile typical of strong flours characterized by high FS (from 9 to 42.9 min for RF21 and RF17, respectively). Beside FS, flours showed high water absorption (ranging from 61.4 to 71 g/100g for RF10 and RF16, respectively; data not shown) and long development time (from 6.1 to 33.7 min for RF6 and RF9, respectively; data not shown), suggesting high quality gluten and good bread-making performance.

Dough stability index - expressing the length of time from the arrival of the maximum torque line to 500 BU to the departure of the maximum torque line from 500 BU - provides information on dough resistance to prolonged mixing: the higher the FS, the stronger the gluten network. Flours with FS greater than 16 min are considered the most suitable raw material for manufacturing highly leavened products, which requires long fermentation time (Foca et al., 2007).

In Table 1 are also summarised the calculated indices from the GlutoPeak profiles of refined flours; whereas the latter are presented in Fig. 1 together with the related whole grain samples profiles. During the test, the sample slurry is subjected to intense mechanical action promoted by the speed of the rotating element. The increase in torque corresponds to the formation of the gluten network. After reaching a maximum value, the torque curve declines, due to prolonged mixing at high speed which causes the breakage of gluten network (Marti, Cecchini, D'Egidio, Dreisoerner, & Pagani, 2014). Usually, hard wheat flours exhibit longer aggregation time (i.e. peak maximum time) and higher maximum torque (i.e. peak torque) than flours of soft wheat cultivars (Lu & Seetharaman, 2014), while flours for wafers or batters show very much delayed peak formation and much lower torque (data not shown). More recently, the area under the peak (i.e. energy to peak), which takes into consideration both the indices, has been found suitable for predicting conventional parameters related to dough strength (Marti, Ulrici, Foca, Quaglia, & Pagani, 2015). To the best of our knowledge, this is the first study exploring the gluten aggregation profile of hard spring varieties. Spring wheat samples showed a faster aggregation (i.e. lower PMT), higher MT, and a broader peak than winter wheats (Marti, Augst, Cox & Koehler, 2015). The use of different versions of the software makes the energy data somewhat difficult to compare with winter wheat. For spring wheat varieties here considered, energy to peak ranges from 1485 to 3843 AU for RF18 and RF9 varieties, respectively. A moderately correlation ($r = 0.59$; $p = 0.005$) was found between this index and FS. The software also provides the aggregation energy, expressed in GPU, which is the area under the curve between 15 s before and 15 s after the peak. However, for this set of samples, this parameter was not significantly correlated with FS. Indeed, looking at the GlutoPeak profile, most of the curves exhibited a very broad peak, instead of a sharp one (Fig. 1). Thus, for this kind of shape, the area under the curve till 15 s after peak (i.e. EnPM) should be considered, being moderately correlated ($r = 0.62$; $p = 0.0019$) with FS.

Whole grain flour showed a rapid build up in consistency to a sharply defined peak followed by a rapid break down, while the related refined flour showed a much slower build up in dough consistency and a relatively more time to achieve peak consistency (Fig. 1).

Concerning whole grain profiles, a high MT and a low PMT are observed and resulted in an overall low aggregation energy, suggesting a weak gluten network. A similar trend in gluten aggregation profile has been found adding fiber-rich raw materials to refined wheat flour (Marti, Torri, Casiraghi, Franzetti, Limbo, Morandin, Quaglia, & Pagani, 2014; Marti, Qiu, Schoenfuss, & Seetharaman, 2015). This behaviour is likely due to gluten dilution, accounting for the decrease in energy and the fast aggregation. On the other hand, the increase in MT could be related to either the ability of fiber to absorb water or the higher kernel protein content compared to refined flours. Indeed, it has been observed previously that increasing protein content of wheat flour led to an increase in torque (Marti, Augst, Cox, & Koehler, 2015; Marti, Ulrici, Foca, Quaglia, & Pagani, 2015).

3.2 Multivariate approach

This work proposes an innovative approach for GlutoPeak data, which intends to highlight interesting information without any index calculation. Such a multivariate data processing could be of particular interest when considering whole grain analysis, for which a specific index value could give a misleading information due to peculiar GlutoPeak profile generated and the lack of background in the whole grain analysis by GlutoPeak test.

Until now, a chemometric approach was applied only to evaluate together all the discrete indices traditionally calculated on the GlutoPeak curve (Marti, Ulrici, Foca, Quaglia, & Pagani, 2015); in the present study, a further step was introduced, carrying out PCA directly on the profiles.

3.2.1 Refined flours: data exploration

Fig. 2 compares PCA results of the two approaches (discrete indices vs. whole curves): Fig. 2a and Fig. 2b are, respectively, the score and the loading plot obtained considering the five most used indices (PMT, MT, EnMT, EnPM and AgrEn); Fig. 2c and Fig. 2d are the score plot and the loading plot of the profiles. The samples in both of the score plot are coloured according to a chromatic scale that is proportional to the FS value, from blue – for low FS value – to red – for high farinographic stability. The score plot calculated from the five indices matrix shows a trend according to the FS values, indeed samples with low FS are arranged in the left-bottom quarter (dark blue samples) whereas samples with FS values higher than 23.5 min are in the right-top quarter with the exception of sample RF19 (Fig. 2a). Comparing the score plot, the evaluation of the whole profile (Fig. 2c) allows better highlighting of a trend, from the left-bottom to the right-top corner, in the orthogonal space; also in this case sample RF17 appears as an outlier. All the samples with FS higher than 17.5 min have positive PC1 scores except sample RF17 (Figure 2c), suggesting a boundary between two classes (FS>17.5 min and FS<17.5 min) to be used for further classification approaches. A detailed analysis of loading plots, in comparison with the corresponding score plots, allows a deeper understanding the relationships among variables and between variables and samples.

In particular, for the indices (Figure 2b), the loading plot shows associated discrete variables that are positively correlated in terms of useful information (AgrEn and MT, EnMT and EnPM). It is possible to notice that AgrEn and MT are positioned in the right-bottom quarter, thus they stretch samples that have positive PC1 values and negative PC2 values in the score plot; whereas EnMT and EnPM are in the right-top of the loading plot, contributing to split samples with high FS values (> 30 min) from the others. PMT shows a different behaviour as it is located in the left-top of the loading plot, the same region where it is possible to find samples RF11, RF15 and RF18. Combining the loading information and the fact that these samples have central FS values in respect to the analysed set, it is plausible to believe that this index is not particularly correlated with sample grouping according to FS characteristic.

The loading plot of the first two principal components along time (Fig. 2d) highlights the two most important regions of the GlutoPeak profiles: around 75 s, loadings exhibit high positive values on PC1 and negative values on PC2, whereas, around 150 s, an inverse trend is observed. By comparison with the GlutoPeak profiles, it is possible to notice that the changes highlighted by PCA loadings are linked to the average time of the beginning of gluten aggregation, i.e. the maximum peak slope (75 s), and the average time before torque falling off when gluten breaks down (150 s). Thanks to the joint interpretation of scores and loadings, it is possible to notice that the horizontal shift along the time axis, characterizing the very broad peaks of flour profiles, is associated with different FS values: peaks shifted towards longer stability time are associated with samples with FS values higher than 17.5 min, while earlier peaks are associated to FS values lower than 17.5 min. In other words, the joint analysis confirms what was already commented by the scores evaluation: samples with FS values lower than 17.5 min are located in the right-bottom corner of the PC score space, characterized by positive scores on PC1 and negative scores on PC2, which correspond to the relative loading intensities of the peak at 75 s. On the contrary, samples located towards the left-top corner are associated with a delayed peak (around 150 s), as evidenced by the loading trend. Thus, it is possible to assess that PCA using the GlutoPeak profile gives thorough information about samples considering their FS, bypassing the calculation of specific indices, which, in some case (i.e. PMT) could be not that informative in respect to the studied property and doing the groundwork for sample classification.

3.2.2 Whole grain: data exploration

The same approach tested for the GlutoPeak profiles of refined flour was performed to verify if it is possible to extract relevant information about dough properties directly from whole grain samples without a refining process. Therefore, PCA was carried out and the outcomes are presented in Fig. 3. In the score plot (Fig. 3a) a trend similar to that observed for refined flour samples can be observed, although less evident and mainly ascribable to PC1. In particular, whole grain flour from samples with FS values higher than 17.5 have negative PC1 scores, confirming the classes boundary forecast by PCA on refined flour GlutoPeak profiles. Regarding the loading plot (Fig. 3b), only one interesting peak could be highlighted, around 40 s. Indeed, the peak characterizing PC1 loadings describes differences between samples linked to the high torque and the shift of the peak occurring around 40 s in the GlutoPeak, also associated with torque intensity, suggesting that the higher the peak for whole grain flours, the lower the FS value. Indeed, in whole grain samples, MT was significantly correlated to bran content ($r = 0.62$; $p = 0.0019$), that negatively affect dough formation and its strength during mixing, decreasing FS.

PCA confirmed to be a reliable method to explore the variance hidden in the data. In this case, the main variables linked to samples differentiation were identified directly on the whole grain GlutoPeak profile, allowing us to bypass calculation of indices that could lead to controversial conclusion on the gluten aggregation properties of the final product.

3.5 Refined flours and whole grain: classification

On the basis of the outcomes obtained from the exploratory study, the final aim of this work was to classify hard red spring wheat samples according to FS value using the whole GlutoPeak curves. To perform a supervised classification, it is necessary to define a-priori classes using a FS cut-off; since in the PCA score plots of both refined and whole grain flours it is identifiable a sample grouping linked to PC1 values, two classes were defined setting as threshold 17.5 min of FS.

In the choice of the best K-NN classification rule, several parameters were considered, including data pre-processing (raw data, standard normal variate transform, first- and second-order derivatives, with the Savitzky-Golay method, third order polynomial, 11 datapoint window), distance (Euclidean, Mahalanobis) and number of K neighbors (odd values from 1 to 7). All of the combinations were evaluated, looking for the highest classification rate in fitting. The best conditions, in term of classification rate in fitting, were found for raw data, Euclidean distance and K = 1. The reliability of the method was tested by leave-one-out cross-validation expressing results as misclassification matrix and related prediction rate (Table 2).

Although sample trends within the score plot were less evident for whole grain samples, comparable results were obtained in term of average prediction ability (81.8%); membership attribution is more balanced – in term of prediction rate of the two categories - using refined flour curves while, with whole grain data, it is more effective at predicting samples with high FS values. In particular, the classification model built for flour samples performed well in discriminating samples of both classes, missing less than 21% of the samples no matter the considered class. The whole grain model performed better in identifying samples with FS values higher than 17.5 min, indeed 13 samples out of 14 were correctly recognized as member of class 1; whereas class 2 prediction ability was 62.5 %. Sample 17, in both whole grain and refined flour models, resulted misclassified. Even in the PCA results it behaved as an outlier, however it was not removed from the classification analysis as the number of samples was already low.

4. CONCLUSIONS

The multivariate analysis of gluten aggregation kinetics of hard red spring wheat varieties highlighted that the GlutoPeak test is able to classify wheat according to dough stability, i.e. the farinographic index widely used for defining wheat end-uses according to gluten strength.

In addition, wheat classification can be obtained by analysing directly the GlutoPeak curves of the whole grains flour, skipping the conventional milling process to obtain the refined flour.

The use of GlutoPeak test as a rapid small-scale test for wheat classification on whole grain flour could have a tremendous impact on breeders and the milling industry because it requires only a small sample and is characterized by rapidity, reliability, and little/absence of technical skill. At the same time, the possibility of obtaining reliable results also on whole grain flours makes the GlutoPeak the potential ideal test for evaluating large numbers of breeder's lines and wheat varieties, thus facilitating quality evaluations at early stages of a breeding program and at the milling receiving station, respectively.

Last but not least, instead of using the indices calculated by the software, the application of multivariate analysis on the curve highlighted that the GlutoPeak profile might “hide” useful information related to gluten strength.

Additional studies are required to confirm these findings on different type of wheat – including soft wheat and hard winter wheat – and on a larger set of samples.

References

Banu, I., & Aprodu, I. (2015). Association of physicochemical with technological properties of wheat. International Journal of Food Science and Technology, 50, 1644-1650.

Dudoit, S., Fridly, J., & Speed, P. (2002). Comparison of discrimination methods for the classification of tumors using gene expression data. Journal of the American Statistical Association, 97, 77–87.

Foca, G., Ulrici, A., Corbellini, M., Pagani, M. A., Lucisano, M., Franchini, G. C., & Tassi, L. (2007). Reproducibility of the Italian ISQ method for quality classification of bread wheats: An evaluation by expert assessors. Journal of the Science of Food and Agriculture, 87, 839-846.

Giovenzana, V., Beghi, R., Malegori, C., Civelli, R., & Guidetti, R. (2013). Wavelength selection with a view to a simplified handheld optical system to estimate grape ripeness. American Journal of Enology and Viticulture, 65, 117-123.

Kaur-Chandi, G., & Seetharaman, K. (2012). Optimization of gluten peak tester: A statistical approach. Journal of Food Quality, 35, 69-75.

Lu, Z., & Seetharaman, K. (2014). Suitability of Ontario-grown hard and soft wheat flour blends for noodle making. Cereal Chemistry, 91, 482-488.

Malegori, C., Marques, E. J. N., de Freitas, S. T., Pimentel, M. F., Pasquini, C., & Casiraghi, E. (2017). Comparing the analytical performances of Micro-NIR and FT-NIR spectrometers in the evaluation of acerola fruit quality, using PLS and SVM regression algorithms. Talanta, 165, 112-116.

Marti, A., Cecchini, C., D'Egidio, M. G., Dreisoerner, J., & Pagani, M. A. (2014). Characterization of durum wheat semolina by means of a rapid shear-based method. Cereal Chemistry, 91, 542-547.

Marti, A., Torri, L., Casiraghi, M. C., Franzetti, L., Limbo, S., Morandin, F., Quaglia, L., & Pagani, M. A. (2014). Wheat germ stabilization by heat-treatment or sourdough fermentation: Effects on dough rheology and bread properties. LWT-Food Science and Technology, 59, 1100-1106.

Marti, A., Qiu, X. Schoenfuss, T. C., & Seetharaman, K. (2015). Characteristics of Perennial Wheatgrass (Thinopyrum intermedium) and refined wheat flour blends: impact on rheological properties. Cereal Chemistry, 92, 434-440.

Marti, A., Augst, E., Cox, S., & Koehler, P. (2015). Correlations between gluten aggregation properties defined by the GlutoPeak test and content of quality-related protein fractions of winter wheat flour. Journal of Cereal Science, 66, 89-95.

Marti, A., Ulrici, A., Foca, G., Quaglia, L., & Pagani, M. A. (2015). Characterization of common wheat flours (Triticum aestivum L.) through multivariate analysis of conventional rheological parameters and gluten peak test indices. LWT-Food Science and Technology, 64, 95-103.

Oliveri, P., & Downey, G. (2012). Multivariate class modelling for the verification of food-authenticity claims. Trends in Analytical Chemistry, 35, 74-86.

Pagani, M. A., Marti, A., & Bottega, G. (2014). Wheat milling and flour quality evaluation. In: Bakery Products Science and Technology, Second Edition, eds W. Zhou, Y. H. Hui, I. De Leyn, M. A. Pagani, C. M. Rosell, J. D. Selman and N. Therdthai. John Wiley & Sons, Ltd, Chichester, UK. pp 17-53.

Pastor, K., Ačanski, M., Vujić, D., Bekavac, G., Milovac, S., & Kravić, S. (2016). Rapid method for small grain and corn flour authentication using gc/ei–ms and multivariate analysis. Food Analytical Methods, 9, 443-450.

Shepherd, L.V.T., Fraser, P., & Stewart, D. (2011). Metabolomics: A second-generation platform for crop and food analysis Bioanalysis, 3, 1143-1159.

Vandeginste, B. G. M., Massart, D. L., Buydens, L. M. C., De Jong, S., Lewi, P. J., & Smeyers-Verbeke, J. (1998). Handbook of Chemometrics and Qualimetrics, Vol. 20B. Elsevier, Amsterdam.

Vidya, S., Ravi, R., &Bhattacharya, S. (2013). Effect of thermal treatment on selected cereals and millets flour doughs and their baking quality. Food and Bioprocess Technology, 6, 1218-1227.

Figure Captions

Figure 1. GlutoPeak profiles of whole grain flours (blue dashed lines) and refined flours (black straight lines).

Figure 2. Principal Component Analysis on refined flour data. (a) Score plot and (b) loading plot obtained considering the five most used GlutoPeak indices (PMT, MT, EnMT, EnPM and AgrEn); (c) Score plot and (d) loading plot calculated from the GlutoPeak curves. Samples in both of the score plots are coloured according to a chromatic scale that is proportional to the farinographic stability (FS) value, from blue – for low FS values – to red – for high FS values.

AgrEn, Aggregation Energy; EnMT, Energy to Maximum Torque; EnPM, Energy after Maximum Torque; MT, Maximum Torque; PMT, Peak Maximum Time.

Figure 3. Principal Component Analysis on whole grain data. (a) Score plot and (b) loading plots obtained considering the the GlutoPeak curves. Samples in the score plot are coloured according to a chromatic scale that is proportional to the farinographic stability (FS) value, from blue – for low FS values – to red – for high FS values.

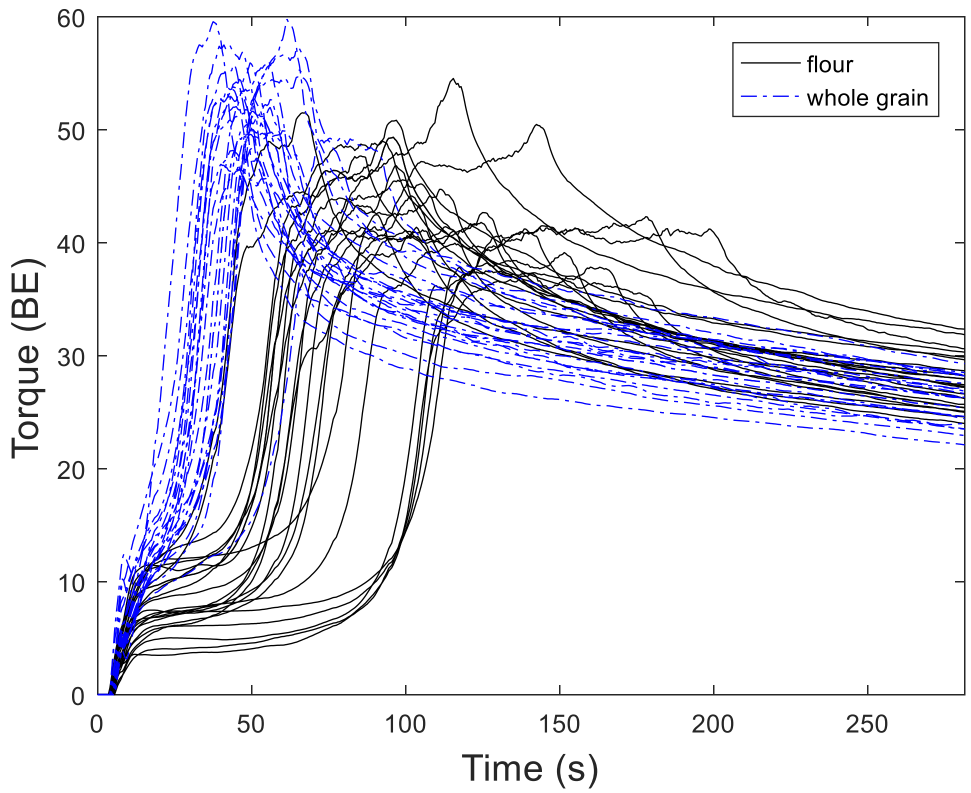

Figure 1: GlutoPeak profiles of whole grain flours (blue dashed lines) and refined flours (black straight lines).

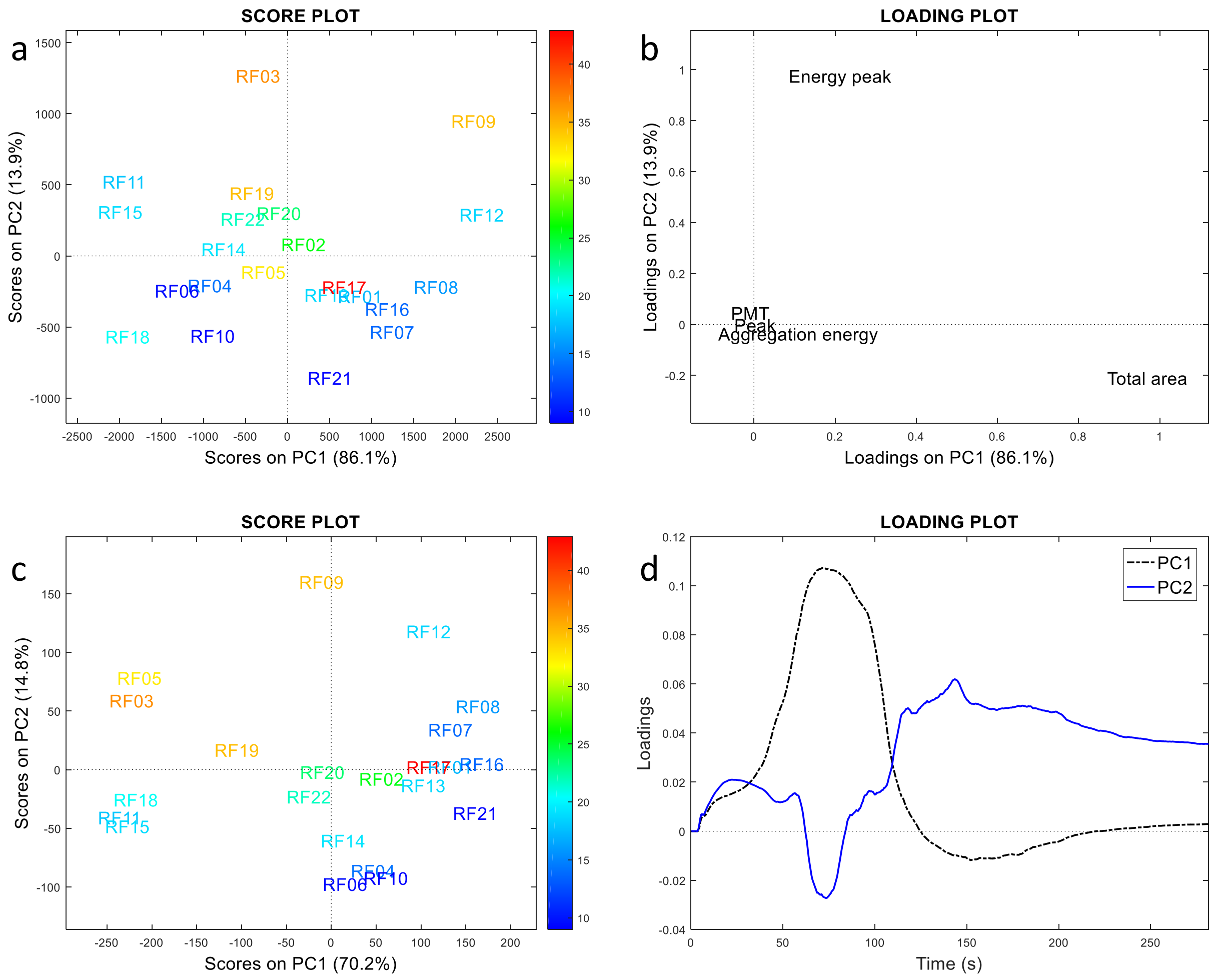

Figure 2. Principal Component Analysis on refined flour data: a) scores plot obtained considering the five most used indices (PMT, MT, EnMT, EnPM and AgrEn); b) loadings plot obtained considering the five most used indices (PMT, MT, EnMT, EnPM and AgrEn); c) and d) scores plot and loadings plot calculated from the GlutoPeak profiles. The samples in both of the scores plot are coloured according to a chromatic scale that is proportional to the FS value, from blue – for low FS value – to red – for high farinographic stability.

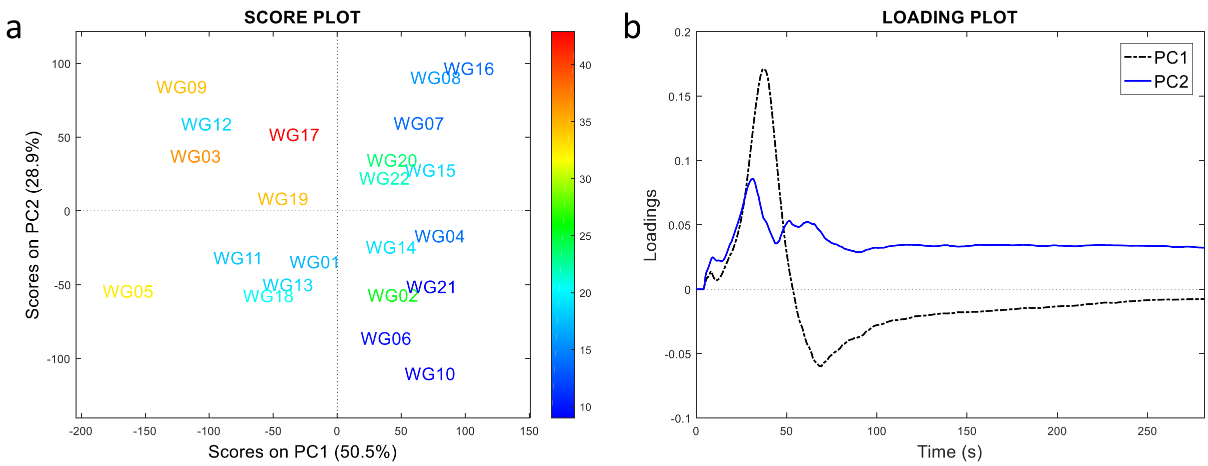

Figure 3. Principal Component Analysis on whole grain data: a) scores plot obtained considering the the GlutoPeak profiles; b) loadings plot calculated from the GlutoPeak profiles. The samples in both of the scores plot are coloured according to a chromatic scale that is proportional to the FS value, from blue – for low FS value – to red – for high farinographic stability.