# Characterization of common wheat flours (*Triticum aestivum* L.) through multivariate analysis of conventional rheological parameters and Gluten Peak Test indices

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**ABSTRACT**

The GlutoPeak consists in high speed mixing of a small amount of wheat flour (<10 g) added with water, and in registering a torque vs. time curve in a very short time (<10 min). Peak torque, peak maximum time, and energy values are calculated from the curve, and used to estimate the aggregation behavior of gluten. The information brought by the GlutoPeak indices is still difficult to interpret correctly, also in relation to the conventional approaches in the field of cereal science. A multivariate approach was used to investigate the correlations existing between the GlutoPeak indices and the conventional rheological parameters. 120 wheat flours- different for protein, dough stability, extensibility, tenacity, and strength, and end-uses - were analyzed using the GlutoPeak and conventional instrumentation. The parameters were subjected to a data exploration step through Principal Component Analysis. Then, multivariate Partial Least Squares Regression (PLSR) models were developed using the GlutoPeak indices to predict the conventional parameters. The values of the squared correlation coefficients in prediction of an external test set showed that acceptable to good results ($0.61 \leq R^2_{PRED} \leq 0.96$) were obtained for the prediction of 18 out of the 26 conventional parameters here considered.

**Keywords:** Wheat Flour; GlutoPeak; Rheological Parameters; Multivariate analysis; Partial Least Squares Regression

**Abbreviations:** Alv-W, Alveographic strength; Alv-P, Alveographic tenacity, Alv-L, Alveographic extensibility; Alv-P/L, Alveographic tenacity; AU, Arbitrary Unit; BE, Brabender Equivalent; Ext_45En, Extensographic energy (45 min); Ext_90En, Extensographic energy (90 min); Ext_135En, Extensographic energy (135 min); Ext_45Ext, Extensographic extensibility (45 min); Ext_90Ext, Extensographic extensibility (90 min); Ext_135Ext, Extensographic extensibility (135 min); Ext_45Max, Extensographic maximal resistance to extension (45 min); Ext_90Max, Extensographic maximal resistance to extension (90 min); Ext_135Max, Extensographic maximal resistance to extension (135 min); Ext_45Rat, Extensographic Ratio (45 min); Ext_90Rat, Extensographic Ratio (90 min); Ext_135Rat, Extensographic Ratio (135 min); Ext_45RatMax, Extensographic Ratio Max (45 min); Ext_90RatMax, Extensographic Ratio Max (90 min); Ext_135RatMax, Extensographic Ratio Max (135 min); Ext_45Res, Extensographic resistance to extension (50 mm; 45 min); Ext_90Res Extensographic resistance to extension (50 mm; 90 min); Ext_135Res, Extensographic resistance to extension (50 mm; 135 min); Far-Abs, Farinographic Water Absorption; Far-Dev, Farinographic Dough development time; Far-Stab, Farinographic Stability; FN, False Negative; FP, False Positive; FU, Farinograph Unit; LV, Latent Variables; GP-En, GlutoPeak Energy; GP-PmaxT, GlutoPeak Peak Maximum Time; GP-Ptor, GlutoPeak Maximum Torque; PCA, Principal Component Analysis; PLSR, Partial Least Squares Regression; Prot, protein content; $R^2_{CAL}$, squared correlation coefficient referred to the calibration of the training set; $R^2_{CV}$, squared correlation coefficient in Cross-Validation; $R^2_{PRED}$, squared correlation coefficient for the prediction of the external test set; RMSE, Root Mean Square Error; RMSEC, Root Mean Square Error in Calibration of the training set; RMSECV, Root Mean Square Error in Cross-Validation; RMSEP, Root Mean Square Error in Prediction of the external test set; TN, True Negative; TP, True Positive; VIP, Variable Importance in Projection.

## 1. Introduction

Common wheat (*Triticum aestivum L.*) is used in a wide range of applications ranging from bread, pastries, biscuits and cakes to noodles and pasta. The functionality and versatility of flour is associated with the capacity of its storage proteins - gliadins and glutenins - to form gluten. Although each wheat flour can organize its storage proteins into a viscoelastic network, its characteristics can greatly differ according to genotype and environmental conditions (Gupta, Batey, & MacRitchie, 1992; Hasniza, Wilkes, Uthayakumaran, & Copeland, 2014). Therefore, different classes of wheat are suited for different types of products to deliver certain functional attributes. For example, flours from strong wheat varieties are preferred for bread where a strong gluten network is desired. On the other hand, soft wheat is preferred for cookies and cakes, where a weak gluten network is desirable. The technological behavior of flour is not only linked to the protein and gluten content, but it is also the result of complex interactions between macromolecules that are responsible for dough performances. Consequently, flour classification is expressed by several parameters, usually measured by rheological approaches that generally provide a quantitative description of mechanical properties (Dobraszczyk & Morgenstern 2003). Attempts to describe the physical properties of doughs have resulted in the design of many rheological devices. Some of these instruments were designed to determine, for instance, the amount of mixing that dough requires or the amount of water that should be added to the flour to obtain dough of the desired consistency (e.g. Farinograph by Brabender®). Others simulate the rounding, and molding in the baking process and measure the dough resistance to uniaxial extension (Extensograph by Brabender®) or to the 3-D extension (Alveograph by Chopin Technologies), in order to determine the dough strength properties useful for predicting bread-making quality. Finally, the Mixolab by Chopin Technologies is a quite new instrument used to characterize the rheological behavior of dough subjected to the simultaneous action of mixing and temperature (Dubat, 2013). The rheological tests - currently used in research laboratories and companies operating in the sector - together with their points of strength and weaknesses, are summarized in Table 1. Although the rheological properties of wheat are considered of great importance for determining baking quality and useful tools for predicting process efficiency (e.g. dough yield, leavening conditions, and so on) and product quality (e.g specific volume, textural attributes) (Olivier & Allen, 1992; Dowell et al., 2008; Mondal & Datta 2008; Ktenioudaki, Butler, & Gallagher, 2010; Banu, Stoenescu, Ionescu, & Aprodu, 2011), most of the procedures are time consuming and require a large amount of samples. The GlutoPeak has been recently proposed for the evaluation of wheat flour quality by measuring the aggregation behaviour of gluten (Kaur Chandi & Seetharaman, 2012). The test has been also proposed as a valid screening tool for durum wheat quality (Mart, Seetharaman, & Pagani, 2013; Marti, Cecchini, D'Egidio, Dreisoerner, & Pagani, 2014). The GlutoPeak indices were significantly correlated with the conventional parameters used for durum wheat characterization and pasta-quality prediction, with the advantages of requiring few minutes of analysis (5-10 minutes) and small amount of sample (9 g). These characteristics are of great interest not only in the durum value chain but also in common wheat sector, and especially in breeding programs. During the test, the sample is mixed with water (flour : water ratio equal to 0.9 : 1) and subjected to intense mechanical action, due to the high speed of the rotating element (set at a constant value between 1900 and 3000 rpm). These conditions - allowing for the formation of the gluten network- initially promote a strong increase in the consistency of the slurry, until reaching a maximum value. Then, the continuous mechanical stress causes the breakdown of the gluten network, which is recorded as a decrease in consistency.

In this study, a large number of wheat flour samples - characterized by different end-uses - was analyzed both considering the chemical and rheological indices conventionally used in the cereal chain (protein content and Farinograph, Alveograph and Extensograph parameters) and the indices derived from the new GlutoPeak test. In order to investigate the correlations existing between the conventional rheological parameters and the GlutoPeak indices, a multivariate statistics-based approach was used, consisting in a data exploration step through Principal Component Analysis (PCA) (Cocchi et al., 2004; Bro & Smilde, 2014), followed by the development of multivariate calibration models using Partial Least Squares Regression (PLSR) (Wold, Sjöström, & Eriksson, 2001; Foca, Masino, Antonelli, & Ulrici, 2011). Moreover, the possibility of using the GlutoPeak indices for the assessment of the wheat flour quality category was also investigated, through the comparison between the class assignments made by the miller on the basis of the Alveograph W values and the corresponding assignments made using the W values predicted by the PLSR model.

## 2. Materials and Methods

### 2.1. Materials

A set of 120 commercial wheat flours were provided by Molino Quaglia S.p.A. (Vighizzolo D'Este, PD, Italy). The samples used in this study are blends of varieties of the 2012-2013 growing season, and are representative of the commercial flours that are actually produced by the miller in order to reach the quality standards required by the market.

### 2.2 Empiric rheological tests

Protein content was measured according to the standard AACC method (AACC 39-11.01, 2000). Mixing profile was determined using the Farinograph-E (Brabender GmbH and Co KG, Duisburg, Germany) equipped with a 300 g mixing bowl (AACCI 54–21, 2000). The following indices were considered: *i)* Water absorption (g/100g) - corresponding to g of water/100 g flour to reach the optimal consistency (500 Farinographic Units, FU); *ii)* Dough development time expressed in minutes - defined as the interval from the first addition of water to the point in maximum consistency range immediately before the first indication of weakening; *iii)* Stability expressed in minutes - defined as the time difference between the point where the top curve first intersects 500-FU and the point where the top curve leaves 500-FU line.

Three-dimensional extension properties of dough were determined by the Alveograph (Chopin, Villeneuve-la-Garenne Cedex, France) according to the AACCI method (AACCI 54–

30.02, 2000). The following indices were considered: *i)* P or tenacity (mm $H_2O$) - corresponding to the maximum pressure on deformation; *ii)* L or extensibility (mm) - corresponding to the length of the curve; *iii)* W or strength (*$10^{-4}$ J) - corresponding to the area under the curve; *iv)* P/L ratio.

Dough extensibility at three different rest times (45, 90, and 135 min) was measured using the Extensograph (Brabender GmbH and Co KG, Duisburg, Germany), according to the AACCI method (AACCI 54-10.01). The following parameters were considered: *i)* Resistance to extension, measured 50 mm after the curve has started and related to the elastic properties; *ii)* Maximal resistance to extension; *iii)* Extensibility, which is the length of the curve; *iv)* Energy - corresponding to the area under the curve; *v)* Ratio - corresponding to the ratio between extensibility and resistance after 50 mm of extension; *vi)* Ratio max - corresponding to the ratio between extensibility and maximal resistance to extension.

**2.3 GlutoPeak Test**

The gluten aggregation properties of flours were measured using the GlutoPeak (Brabender GmbH and Co KG, Duisburg, Germany). An aliquot of 9 g of flour was dispersed in 10 ml of solvent. Both double distilled water ($H_2O$) and 0.33 M Sodium Chloride (NaCl) solution were considered, in order to evaluate the possible differences between the results obtained using these two different solvents. In particular, the tests with NaCl were carried out to mimic the conditions used with the Extensograph measurements, which involved the addition of 2 g / 100 g NaCl. Sample and solvent temperature was maintained at 35 °C by circulating water through the jacketed sample cup. The paddle was set to rotate at 3000 rpm and each test was run for 10 min. The main indices automatically evaluated by the software provided with the instrument (Brabender GlutoPeak v.1.1.0) are: *i)* Maximum Torque expressed in Brabender Equivalents (BE) - corresponding to the peak occurring as gluten aggregates; *ii)* Peak Maximum Time expressed in seconds - corresponding to the time at peak torque. In addition, the area under the peak - expressed in arbitrary units (AU) and corresponding to the energy required for gluten aggregation was calculated using Microsoft

Excel 2010 (Microsoft, Redmond, VA). All the measurements were performed in triplicate, and the average of the results was used for further data analysis.

**2.4 Definition of the wheat flour quality classes**

With particular regards to the leavened baked goods, two main categories can be identified as chemical and biological leavening. The latter can be further distinguished according to the method used for the leavening phase: the straight-dough and the sponge-and-dough processes (Pagani, Lucisano, & Mariotti, 2014). In particular, in Italy about 15% of the wheat flour production is dedicated to the preparation of chemically and physically leavened products such as biscuits and cakes, while 70% is addressed to the production of biologically leavened goods such as bread and pizza (www.infofarine.it). Generally, mill companies are used to prepare suitable wheat kernel mixtures in order to obtain flours that satisfy customers' needs. To this aim, the W alveographic index – which is related to flour strength - is generally considered to define the technological behavior of flours. According to this criterion, three types of common wheat flours are in fact identified by the miller (Molino Quaglia S.p.A.) as follows: i) *class 1*: chemically leavened products ($100 *10^{-4}$ J $<W < 130*10^{-4}$ J); ii) *class 2*: straight-dough systems ($180 *10^{-4}$ J $<W < 280 *10^{-4}$ J); iii) *class 3*: sponge-and-dough systems ($W \geq 320*10^{-4}$ J).

The 80% of the flours used in this study belongs to these three categories, whereas the remaining 20% - which is produced by the mill only for specific requests from customers - is characterized by intermediate W values. This distribution is strongly related to the types of flour produced by the mill, whose customers are mainly represented by artisanal and industrial bakers. In fact, the flour samples considered in the present study were collected with the aim of reflecting the properties of the commercial flours that are actually produced by the miller, and not to plan *a priori* the properties of the flour samples to be considered, based on criteria like e.g. their quality classes. In particular, in our study only one sample belongs to class 1; 35 samples belong to class 2; 55 samples to class 1; 9 samples are between class 1 and 2; and 20 samples are between class 2 and 3.

## 2.5 Data Analysis

The whole data were merged into a unique dataset with size {120 × 32}, composed by the values of the 32 chemical and rheological parameters measured on the 120 wheat flour samples. The basic statistics of the dataset are reported in Table 2.

PCA was then used as an unsupervised explorative technique to analyze the whole dataset (using autoscaling as preprocessing), in order to detect the possible presence of outliers and of data clusters corresponding to the different wheat flour categories. Moreover, PCA allowed also to obtain a first overview of the linear correlations existing among the analyzed variables, in particular between the GlutoPeak indices and the other parameters.

Then, for the calculation of the PLSR calibration models, the whole dataset was split into a dataset X with size {120 × 6}, containing the GlutoPeak indices, and a dataset Y with size {120 × 26}, composed by the remainder parameters. Each single parameter determined with the conventional methods ($y_i$ variable corresponding to the i-th column of dataset Y) was considered separately as a dependent variable for the construction of the calibration models. For each $y$ variable, the PLSR models were calculated considering three possible options as for the descriptor variables: all the six GlutoPeak indices, only the three Glutopeak indices measured using water as solvent, and only the three Glutopeak indices measured using the NaCl aqueous solution as solvent. Notwithstanding the very low number of descriptor variables, PLSR was used instead of Multiple Linear Regression (MLR) due to the presence of correlated variables within the X block. Both the X and Y datasets were randomly split into a training set, containing 80 samples (i.e., 2/3 of the objects of the whole dataset), and a test set, containing the remainder 40 samples, to be used for external validation. X and Y variables were preprocessed by autoscaling, and the optimal number of latent variables (LVs) was chosen by minimizing the error in cross-validation (random group cross-validation, with 10 deletion groups and 20 iterations). The selected model was finally validated by means of the test set.

The performance of the calibration models is expressed by the squared correlation coefficient, $R^2$, since this parameter can be used to compare directly models calculated on different response variables. In particular, three $R^2$ values were calculated, i.e., $R^2_{CAL}$ referred to the calibration of the training set, $R^2_{CV}$ referred to the cross-validation results and $R^2_{PRED}$ referred to the prediction of the external test set values (Foca et al., 2011). Moreover, also the Root Mean Square Error (RMSE) statistics was used, which reports the error of the PLS model in the same units of the *y* variable; also in this case, for each model this parameter is reported for the calibration of the training set (RMSEC), for the cross-validation results (RMSECV) and for the prediction of the test set (RMSEP) (Pigani et al., 2011).

In order to evaluate the contribution of the GlutoPeak indices to the calibration models, the Variable Importance in Projection (VIP) scores of the PLSR models were considered. VIP scores constitute a valuable tool to estimate the importance of each variable used in the PLS model, so that they are often used as a variable selection criterion (Chong & Jun, 2005; Ulrici et al., 2013). The criterion adopted to determine whether a certain variable is actually significant is the 'greater than one rule', which derives from the fact that the average of squared VIP scores equals 1; therefore, only those variables whose values are > 1 in the VIP score plot furnish a significant contribution to the corresponding PLS model.

Since the assignment of each sample to the proper wheat flour quality class is made by the miller based on the Alveograph W value, the PLSR model of W was also used for classification purposes, i.e., the original class assignments made by the miller were compared with those made using the W values calculated (for the training set) or predicted (for the test set) by the model. The results were then evaluated though the corresponding confusion table in terms of True Positive rate (TP, i.e., proportion of positive cases that were correctly identified, also referred to as Sensitivity), True Negative rate (TN, i.e., proportion of negatives cases that were classified correctly, also referred to as Specificity), False Positive rate (FP, i.e., proportion of negatives cases that were incorrectly classified as positive) and False Negative rate (FN, i.e., proportion of positive cases that were incorrectly classified as negative).

Data analysis was performed using PLS-Toolbox (v. 7.8.2, Eigenvector Research Inc., USA), together with some routines written *ad-hoc* in Matlab language (ver. 7.12, The Mathworks Inc., USA).

## 3. Results and Discussion

### 3.1 PCA on the whole dataset

The structure of the whole dataset was explored by means of PCA: a 2 Principal Components (2 PCs) model was obtained, explaining 75% of the whole data variance. The PC1 vs. PC2 score plot is reported in Fig. 1, showing that the wheat flour quality classes are mainly separated along PC1, which accounts by itself for 58% of data variance. In particular, the only sample belonging to class 1 is positioned at the lower value of PC1 and is quite well separated from the "between class 1 and 2" samples, which in turn form a quite compact cluster, adjacent to the cluster of class 2 samples. These latter ones are instead partially superimposed to the samples belonging to class 3, and the "between class 2 and 3" samples lie as expected between the respective upper and lower classes, with a quite high degree of superimposition. The gradual variation of the positions of samples with increasing quality class and the partial superimposition of the classes is not surprising, since wheat flour quality is a complex property that varies in a continuous manner and actually relies on several physical, chemical and rheological characteristics, so that the univocal and certain attribution of a given sample to a quality class is not straightforward at all, and the definition of "wheat quality class" by itself is still a debated problem (Foca et al., 2007). This consideration is confirmed by the corresponding loading plot, reported in Fig. 2, which shows that almost all the variables contribute significantly to PC1, with positive values. This means that in general flour wheat strength is correlated with increasing values of almost all the measured parameters. A further differentiation among the analyzed samples is observed along PC2 (17% explained variance), and can be mainly ascribed to two groups of variables. The former one, at positive values of PC2, corresponds to Farinograph water absorption (Far-Abs), protein content (Prot), and GlutoPeak maximum torque expressed in Brabender Equivalents measured both using water and NaCl solution (GP-Ptor-$H_2O$ and GP-Ptor-NaCl, respectively). The second group of variables, at negative values of PC2, is composed by the GlutoPeak peak maximum time (GP-MaxT-NaCl and GP-MaxT-$H_2O$ for measurements made with water or NaCl solution, respectively), and by the Extensograph ratio between extensibility and resistance measured after 90 and 135 min (Ext_90Rat and Ext_135Rat, respectively). Interestingly, GlutoPeak indices contribute significantly both to PC1 (mainly as for the area under the peak, i.e., GP-En-NaCl and GP-En-$H_2O$), and to PC2.

Concerning the comparison between the GlutoPeak measurements made using water and those made using the NaCl aqueous solution, Fig. 2 highlights the presence of three couples of GlutoPeak indices, suggesting that the change of solvent does not significantly affect the results.

**3.2 PLSR models**

The results of the PLSR calibration models of the 26 reference parameters calculated using all the 6 GlutoPeak indices are reported in Table 3 in terms of model dimensionality (i.e., number of selected latent variables, LVs), RMSE and $R^2$ statistics. On the whole, considering the $R^2_{PRED}$ values, acceptable to good results ($R^2_{PRED} \geq 0.6$) were obtained for 18 out of the 26 considered parameters. As expected, GlutoPeak indices are well correlated with the total protein content ($R^2_{PRED} = 0.91$). The values of the GlutoPeak maximum torque expressed in Brabender Equivalents (GP-Ptor-$H_2O$ and GP-Ptor-NaCl) are the only variables with significant VIP score values (equal to 2.5 for both), confirming what was already observed in the loading plot of Fig. 2.

The best overall performance was obtained for the prediction of Farinograph water absorption ($R^2_{PRED} = 0.96$), whose *y* predicted vs. *y* experimental plot is reported in Fig. 3a. The value of the Root Mean Square Error in Prediction of the external test set obtained by the PLSR model of Far-Abs (RMSEP = 0.44%, *see* Table 3) is comparable with the value of the average experimental error (equal to 0.24%). This latter value was calculated as the square root of the ANOVA within-sample mean square value, using five replicate experimental measurements made on a subset of flour samples (data not reported for conciseness reasons). The model prediction error and the experimental error values are comparable each other, which can be considered as satisfactory. In fact, this means that GlutoPeak can provide estimates of Farinograph water absorption with an uncertainty that is only slightly higher than the uncertainty of the reference method, and in much shorter times.

The VIP score plot reported in Fig. 3b shows that the GlutoPeak indices that essentially contribute to the calibration model of Farinograph water absorption are the same parameters that were selected for total protein content (GP-Ptor-$H_2O$ and GP-Ptor-NaCl, with equal importance) coherently with the PCA results. The correlation between the peak torque (GlutoPeak test) and the water absorption (Farinograph test) can be likely related to the fact that both the indices are strongly associated with the protein content (Holas & Tipples, 1978, Tipples, Meredith, & Holas, 1978).

Among the other Farinograph parameters, also stability is well predicted ($R^2_{PRED}$ = 0.88); in this case, based on the VIP score values, the significant variables are GP-En-NaCl (VIP = 1.6) and GP-En-$H_2O$ (VIP = 1.7) and, to a minor extent, GP-PMaxT-NaCl (VIP = 1.2). Flour samples which exhibit great resistance to mechanical stresses - as those exerted during the GlutoPeak test (3000 rpm) – will show great stability during mixing under gentle conditions as those occurring in the Farinograph bowl (63 rpm) and for prolonged time.

As for Farinograph Dough development time, it has not been possible to obtain an acceptable estimate based on the GlutoPeak indices. Indeed, the two tests here considered (Farinograph and GlutoPeak) are carried out using different hydration conditions: in the Farinograph a dough mass (53.1-62.9 g water/100 g flour) is prepared and a certain time is necessary to homogeneously distribute water among flour components, while in the GlutoPeak a slurry (111 g water/100 g flour) is obtained.

Among the Extensograph parameters, for all the three considered measurement times (45, 90 and 135 min) satisfactory models have been obtained for Energy and Max resistance to extension. Interestingly, for both these parameters the VIP score values are very similar, and show almost the same variations with the different measurement times, as it is reported in Fig. 4. This is related to the characteristics of the flours analyzed in the present study. According to the farinographic and alveographic indices, most of them are defined as "strong" flours whose extensibility features do not worsen over time (Table 2), in agreement with their end-uses such as processing that requires long fermentation time (straight-dough or sponge-and-dough systems). GP-En-$H_2O$ and GP-En-NaCl play always the major role, but with increasing the measurement time, also GP-PmaxT-NaCl assumes a statistically significant contribution to the calibration models. Quite acceptable performances have been obtained also for Extensibility, considering the high experimental errors that generally affect this parameter (the average error of replicate experimental measurements being equal to about 5 mm). In particular, the best results have been obtained for measurements at 90 and at 135 min. For these points (90 and 135 min) also the calibration models of Resistance to extension and of Ratio max were acceptable. This behavior can be likely explained by the protein polymerisation occurring during resting (Weegels, van de Pijpekamp, Graveland, Hamer, & Schofield, 1996; Borneo & Khan, 1999).

Concerning the Alveograph parameters, it was not possible to estimate L ($R^2_{PRED}$ = 0.05) – which is related to dough extensibility - and, consequently, also its derived parameter P/L ($R^2_{PRED}$ = 0.32). Conversely, in the evaluation of the performance of the calibration models for W ($R^2_{PRED}$ = 0.73) and P ($R^2_{PRED}$ = 0.86) – related to dough strength and tenacity, respectively - it must be noticed that since these rheological parameters are highly operator dependent, they are affected by an experimental error that may be as high as 10% of the mean value (Foca et al., 2007). In view of this fact, the RMSE values obtained for W and P indicate that these models can be considered as quite satisfactory. As far as Alveograph W is concerned, based on the VIP score values, the statistically significant Glutopeak indices are GP-Ptor_$H_2O$ and GP-Ptor-NaCl (VIP = 1.6 and 1.4, respectively) and GP-En-$H_2O$ and GP-En-NaCl (VIP = 1.1 and 1.4, respectively). The same indices are the significant ones also for Alveograph P, where GP-Ptor_$H_2O$ and GP-Ptor-NaCl (VIP = 1.8 and 1.6, respectively) are both more significant than GP-En-$H_2O$ and GP-En-NaCl (VIP = 1.1 and 1.3, respectively). The W values obtained by the PLSR model reported in Table 3 were also used to assign the samples to the different quality classes described in Section 2.4, and the quality class assignments of both the training set and the test set objects were compared with the corresponding assignments made by the miller using the original W values. The results of this comparison, reported in Table 4, show that in general the class assignments made using the GlutoPeak indices + PLSR match acceptably those made by the miller (*see* section 2.4); the greatest errors are observed for the “between class 2 and 3” samples, coherently with what previously observed in the score plot of Fig. 1.

Finally, concerning the comparison between the two solvents used for the GlutoPeak measurements, Table 5 reports the $R^2$ statistics of the PLSR models obtained using only the GlutoPeak indices measured with water and those of the models obtained with the NaCl solution. Moreover, in order to highlight the conditions leading to the overall best performances for each analyzed parameter, the last column of Table 5 reports the indication of the set of GlutoPeak indices that leads to the highest value of $R^2_{PRED}$, considering also the results reported in Table 3 (i.e., with all the six GlutoPeak indices). On the whole, focusing on the 18 parameters leading to at least acceptable models (i.e., with $R^2_{PRED} \geq 0.6$), for 8 parameters the best results were obtained considering all the six GlutoPeak indices, for other 8 parameters the best results were obtained with the three GlutoPeak indices measured using water as solvent, and only for 2 parameters the best results were obtained using the three Glutopeak indices measured using the NaCl aqueous solution. Considering that the use of all the six indices requires the execution of two subsequent GlutoPeak runs (one with water and one with NaCl solution), and since the differences between the $R^2_{PRED}$ values obtained with all the six indices and those obtained using only the three indices measured using water are however small (the highest difference is equal to 0.05 for Farinograph Stability), this comparison suggests that performing a unique GlutoPeak run using water as solvent could be enough to gain at least an acceptable preliminary estimate of the main chemical and rheological parameters used to define wheat flour behavior.

## 4. Conclusions

The results obtained from the screening of 120 commercial wheat flours are encouraging in showing GlutoPeak test as a fast and reliable approach for predicting wheat dough performances and thus flour end-use. The use of multivariate statistics demonstrated that GlutoPeak indices were significantly correlated with many of the conventional parameters which are currently used for flour characterization, with the advantages of requiring few minutes of analysis (less than 10 min) and a small amount of sample (9 g), properties of great interest along the value chain. Furthermore, through the use of the PLSR model for the prediction of the Alveograph W values, the GlutoPeak indices also allowed to obtain an acceptable assessment of the wheat flour quality categories. Among the three GlutoPeak indices that were considered in this study, the energy value and the maximum torque generally resulted the most significant ones for the prediction of the conventional parameters related to dough mixing stability, extensibility, and tenacity. As regards the type of solvent to employ for GlutoPeak measurements, calibration results showed that using water is sufficient to obtain satisfactory estimates of the conventional parameters values, allowing a faster experimental procedure with no need to prepare NaCl solutions.

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## Captions to Tables and Figures

**Table 1.** Rheological approaches currently used for flour characterization

**Table 2.** Basic statistics of the 32 chemical and rheological parameters.

**Table 3.** Results of the PLSR calibration models of the 26 reference parameters calculated using all the 6 GlutoPeak indices.

**Table 4.** Class assignments made using the PLSR model of Alveograph W. *Class 1*: chemically leavened products ($100 *10^{-4}$ J <W < $130*10^{-4}$ J); *Class 2*: straight-dough systems ($180 *10^{-4}$ J <W < $280 *10^{-4}$ J); *Class 3*: sponge-and-dough systems (W ≥ $320*10^{-4}$ J). For each class, the following statistics are also reported: TP% = true positives, i.e., percentage of correctly identified samples; TN% = true negatives, i.e., percentage of correctly rejected samples; FP% = false positives; i.e., percentage of incorrectly identified samples; FN% = false negatives, i.e., percentage of incorrectly rejected samples.

**Table 5.** Comparison between the performances of the PLSR models calculated using all the six GlutoPeak indices (*"all indices"*), only the three GlutoPeak indices measured using water as solvent (*"$H_2O$"*), and only the three Glutopeak indices measured using the NaCl aqueous solution (*"NaCl"*).

**Figure 1.** PC1 vs. PC2 score plot of the whole dataset; symbols indicate the different wheat flour quality classes.

**Figure 2.** PC1 vs. PC2 loading plot of the whole dataset; symbols indicate the different instrumental techniques.

**Figure 3.** (a) PLSR Predicted vs. experimentally measured values of Farinograph water absorption (g/100g) and (b) corresponding VIP score plot.

**Figure 4.** VIP scores for Extensograph Energy (upper plot) and Max resistance to extension (lower plot).

**Table 1**

| Test | Principle | Time required* | Sample amount required |
|---|---|---|---|
| Farinograph Test | It measures the mixing properties of the dough prepared with the amount of water required for the dough to reach a definite consistency (500 UB) (AACC 54-21; ICC 115/1) | ~50-60 min** | 10g, 50g or 300g |
| Extensograph Test | It measures the stretching properties of the dough under standardized conditions (AACC 54-10; ICC 114/1) | ~150 min | 300 g |
| Alveographic Test | It measures resistance to 3-D extension of a thin sheet of dough, prepared at a constant hydration level (43.3g/100g) (AACC 54-30.02; ICC 121) | ~50-60 min | 250 g |
| Mixolab Test | It measures changes in consistency of dough subjected to the simultaneous action of mixing and temperature (AACC 54-60.01) | ~50-60 min | 50 g |
| GlutoPeak Test | It measures torque and time required for gluten aggregation | ~5-10 min | <10g |

* *including sample preparation and cleaning*

** *including the step for the determination of the optimal water absorption*

# Table 2

| | | Min | Max | Mean* | Median | Standard deviation |
|---|---|---|---|---|---|---|
| GlutoPeak | Peak Maximum Time (s) - $H_2O$ (GP-PmaxT-$H_2O$) | 63.8 | 164.3 | 113.7 | 110.1 | 21.1 |
| | Maximum Torque (BE) - $H_2O$ (GP-Ptor-$H_2O$) | 28.6 | 58.6 | 42.5 | 42.3 | 6.6 |
| | Area under the Peak (AU) - $H_2O$(GP-En-$H_2O$) | 15.1 | 36.1 | 25.8 | 24.9 | 4.1 |
| | Peak Maximum Time (s) - NaCl (GP-PmaxT-NaCl) | 69.7 | 193.6 | 121.2 | 110.4 | 28.8 |
| | Maximum Torque (BE) - NaCl (GP-Ptor-NaCl) | 28.1 | 62.2 | 43.4 | 42.7 | 7.7 |
| | Area under the Peak (AU) - NaCl(GP-En-NaCl) | 14.4 | 35.6 | 25.8 | 24.5 | 5.1 |
| Protein content (g/100g) | | 11.2 | 15.9 | 13.2 | 13.3 | 0.9 |
| Farinograph | Water absorption (%) (Far-Abs) | 53.1 | 62.9 | 57.7 | 57.7 | 2.0 |
| | Dough development time (min) (Far-Dev) | 1.3 | 24.4 | 6.2 | 5.5 | 5.0 |
| | Stability (min) (Far-Stab) | 6.0 | 29.0 | 18.2 | 18.2 | 7.0 |
| Alveograph | W (*$10^{-4}$J) (Alv-W) | 120 | 417 | 295 | 312 | 68 |
| | P/L (Alv-P/L) | 0.27 | 1.17 | 0.70 | 0.70 | 0.15 |
| | P ($mmH_2O$) (Alv-P) | 37 | 98 | 76 | 80 | 11 |
| | L (mm) (Alv-L) | 79 | 161 | 112 | 110 | 14 |
| Extensograph 45 min | Resistance to extension (BU) (Ext_45Res) | 187 | 315 | 264 | 266 | 24 |
| | Max resistance to extension (BU) (Ext_45Max) | 239 | 557 | 434 | 450 | 74 |
| | Extensibility (mm) (Ext_45Ext) | 156 | 223 | 191 | 188 | 17 |
| | Energy ($cm^2$) (Ext_45En) | 61 | 159 | 112 | 115 | 24 |
| | Ratio (Ext_45Rat) | 1.10 | 1.70 | 1.39 | 1.40 | 0.1 |
| | Ratio max (Ext_45RatMax) | 1.40 | 2.90 | 2.26 | 2.30 | 0.27 |
| Extensograph 90 min | Resistance to extension (BU) (Ext_90Res) | 203 | 422 | 313 | 314 | 43 |
| | Max resistance to extension (BU) (Ext_90Max) | 258 | 758 | 53 | 525 | 123 |
| | Extensibility (mm) (Ext_90Ext) | 154 | 228 | 189 | 185 | 18 |
| | Energy ($cm^2$) (Ext_90En) | 64 | 210 | 133 | 132 | 38 |
| | Ratio (Ext_90Rat) | 1.20 | 2.20 | 1.66 | 1.70 | 0.19 |
| | Ratio max (Ext_90RatMax) | 1.50 | 3.90 | 2.81 | 2.80 | 0.49 |
| Extensograph 135 min | Resistance to extension (BU) (Ext_135Res) | 202 | 440 | 321 | 320 | 51 |
| | Max resistance to extension (BU) (Ext_135Max) | 178 | 844 | 548 | 524 | 149 |
| | Extensibility (mm) (Ext_135Ext) | 149 | 220 | 184 | 183 | 16 |
| | Energy ($cm^2$) (Ext_135En) | 60 | 215 | 133 | 123 | 41 |
| | Ratio (Ext_135Rat) | 1.20 | 2.20 | 1.74 | 1.70 | 0.23 |
| | Ratio max (Ext_135RatMax) | 1.50 | 4.30 | 2.97 | 2.90 | 0.62 |

* Mean value of all data. All the measurements for each sample were performed in triplicate

**Table 3**

| Parameter | | LVs | RMSEC | RMSECV | RMSEP | $R^2_{CAL}$ | $R^2_{CV}$ | $R^2_{PRED}$ |
|---|---|---|---|---|---|---|---|---|
| Protein content (g/100g) | | 4 | 0.31 | 0.34 | 0.30 | 0.88 | 0.85 | 0.91 |
| Farinograph | Water absorption (%) (Far-Abs) | 2 | 0.49 | 0.52 | 0.44 | 0.93 | 0.92 | 0.96 |
| | Dough development time (min) (Far-Dev) | 1 | 4.44 | 4.64 | 4.37 | 0.19 | 0.12 | 0.26 |
| | Stability (min) (Far-Stab) | 2 | 2.21 | 2.35 | 2.25 | 0.90 | 0.89 | 0.88 |
| Alveograph | W ($*10^{-4}$J) (Alv-W) | 2 | 26.99 | 28.77 | 37.60 | 0.83 | 0.80 | 0.73 |
| | P/L (Alv-P/L) | 2 | 0.11 | 0.12 | 0.13 | 0.44 | 0.37 | 0.32 |
| | P ($mmH_2O$) (Alv-P) | 3 | 4.65 | 4.94 | 4.36 | 0.83 | 0.81 | 0.86 |
| | L (mm) (Alv-L) | 1 | 12.27 | 12.85 | 17.13 | 0.04 | -0.05 | 0.05 |
| Extensograph 45 min | Energy ($cm^2$) (Ext_45En) | 2 | 11.65 | 12.27 | 11.71 | 0.76 | 0.73 | 0.78 |
| | Resistance to extension (BU) (Ext_45Res) | 3 | 17.12 | 18.25 | 16.77 | 0.49 | 0.42 | 0.46 |
| | Extensibility (mm) (Ext_45Ext) | 2 | 10.55 | 11.13 | 10.83 | 0.59 | 0.54 | 0.64 |
| | Max resistance to extension (BU) (Ext_45Max) | 2 | 35.77 | 38.12 | 36.60 | 0.76 | 0.73 | 0.75 |
| | Ratio (Ext_45Rat) | 3 | 0.14 | 0.15 | 0.14 | 0.09 | -0.04 | -0.09 |
| | Ratio max (Ext_45RatMax) | 3 | 0.19 | 0.21 | 0.17 | 0.51 | 0.43 | 0.53 |
| Extensograph 90 min | Energy ($cm^2$) (Ext_90En) | 2 | 15.13 | 16.08 | 12.80 | 0.84 | 0.82 | 0.88 |
| | Resistance to extension (BU) (Ext_90Res) | 2 | 24.34 | 25.62 | 21.59 | 0.68 | 0.64 | 0.72 |
| | Extensibility (mm) (Ext_90Ext) | 2 | 10.13 | 10.67 | 10.42 | 0.66 | 0.62 | 0.67 |
| | Max resistance to extension (BU) (Ext_90Max) | 2 | 51.36 | 54.61 | 41.25 | 0.83 | 0.80 | 0.88 |
| | Ratio (Ext_90Rat) | 1 | 0.18 | 0.19 | 0.16 | 0.14 | 0.05 | 0.14 |
| | Ratio max (Ext_90RatMax) | 2 | 0.29 | 0.31 | 0.25 | 0.64 | 0.61 | 0.70 |
| Extensograph 135 min | Energy ($cm^2$) (Ext_135En) | 2 | 16.24 | 17.10 | 13.81 | 0.84 | 0.82 | 0.89 |
| | Resistance to extension (BU) (Ext_135Res) | 2 | 25.11 | 26.36 | 30.06 | 0.76 | 0.73 | 0.61 |
| | Extensibility (mm) (Ext_135Ext) | 2 | 9.37 | 9.84 | 11.16 | 0.62 | 0.58 | 0.63 |
| | Max resistance to extension (BU) (Ext_135Max) | 2 | 55.04 | 57.94 | 70.37 | 0.86 | 0.84 | 0.78 |
| | Ratio (Ext_135Rat) | 3 | 0.17 | 0.18 | 0.17 | 0.43 | 0.35 | 0.36 |
| | Ratio max (Ext_135RatMax) | 2 | 0.30 | 0.32 | 0.22 | 0.77 | 0.75 | 0.85 |

**Table 4**

| TRAINING SET | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **Confusion Table** | | | | | | | | | | | |
| | | *predicted as:* | | | | | | | | | |
| | | **class 1** | **> 1 & < 2** | **class 2** | **> 2 & < 3** | **class 3** | **TOTAL** | **TP%** | **TN%** | **FP%** | **FN%** |
| *actual class:* | **class 1** | **1** | 0 | 0 | 0 | 0 | **1** | 100% | 100% | 0% | 0% |
| | **> 1 & < 2** | 0 | **3** | 2 | 0 | 0 | **5** | 60% | 100% | 0% | 40% |
| | **class 2** | 0 | 0 | **19** | 1 | 1 | **21** | 90% | 86% | 14% | 10% |
| | **> 2 & < 3** | 0 | 0 | 4 | **3** | 6 | **13** | 23% | 96% | 4% | 77% |
| | **class 3** | 0 | 0 | 2 | 2 | **36** | **40** | 90% | 83% | 18% | 10% |
| | **TOTAL** | **1** | **3** | **27** | **6** | **43** | **80** | | | | |

| TEST SET | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **Confusion Table** | | | | | | | | | | | |
| | | predicted as: | | | | | | | | | |
| | | **class 1** | **> 1 & < 2** | **class 2** | **> 2 & < 3** | **class 3** | **TOTAL** | **TP%** | **TN%** | **FP%** | **FN%** |
| *actual class:* | **class 1** | **0** | 0 | 0 | 0 | 0 | **0** | - | 100% | 0% | - |
| | **> 1 & < 2** | 0 | **3** | 1 | 0 | 0 | **4** | 75% | 100% | 0% | 25% |
| | **class 2** | 0 | 0 | **12** | 0 | 2 | **14** | 86% | 96% | 4% | 14% |
| | **> 2 & < 3** | 0 | 0 | 0 | **4** | 3 | **7** | 57% | 97% | 3% | 43% |
| | **class 3** | 0 | 0 | 0 | 1 | **14** | **15** | 93% | 80% | 20% | 7% |
| | **TOTAL** | **0** | **3** | **13** | **5** | **19** | **40** | | | | |

**Table 5**

| Parameter | | $H_2O$ GlutoPeak indices | | | | NaCl GlutoPeak indices | | | | Best $R^2_{PRED}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| | | LVs | $R^2_{CAL}$ | $R^2_{CV}$ | $R^2_{PRED}$ | LVs | $R^2_{CAL}$ | $R^2_{CV}$ | $R^2_{PRED}$ | |
| Protein content (g/100g) | | 3 | 0.87 | 0.85 | 0.90 | 3 | 0.87 | 0.86 | 0.90 | All indices |
| Farinograph | Water absorption (%) (Far-Abs) | 2 | 0.91 | 0.90 | 0.95 | 2 | 0.93 | 0.93 | 0.96 | NaCl |
| | Dough development time (min) (Far-Dev) | 3 | 0.25 | 0.17 | 0.24 | 2 | 0.18 | 0.09 | 0.24 | All indices |
| | Stability (min) (Far-Stab) | 3 | 0.90 | 0.88 | 0.83 | 2 | 0.87 | 0.85 | 0.87 | All indices |
| Alveograph | W ($*10^{-4}$J) (Alv-W) | 2 | 0.83 | 0.81 | 0.75 | 2 | 0.79 | 0.77 | 0.70 | $H_2O$ |
| | P/L (Alv-P/L) | 2 | 0.43 | 0.37 | 0.33 | 2 | 0.42 | 0.35 | 0.31 | $H_2O$ |
| | P ($mmH_2O$) (Alv-P) | 3 | 0.82 | 0.80 | 0.87 | 2 | 0.79 | 0.77 | 0.79 | $H_2O$ |
| | L (mm) (Alv-L) | 1 | 0.05 | -0.05 | 0.05 | 1 | 0.04 | -0.06 | 0.04 | $H_2O$ |
| Extensograph 45 min | Energy ($cm^2$) (Ext_45En) | 2 | 0.77 | 0.74 | 0.79 | 2 | 0.71 | 0.68 | 0.73 | $H_2O$ |
| | Resistance to extension (BU) (Ext_45Res) | 3 | 0.47 | 0.41 | 0.41 | 2 | 0.36 | 0.30 | 0.31 | All indices |
| | Extensibility (mm) (Ext_45Ext) | 2 | 0.59 | 0.55 | 0.64 | 2 | 0.56 | 0.51 | 0.62 | $H_2O$ |
| | Max resistance to extension (BU) (Ext_45Max) | 2 | 0.76 | 0.73 | 0.78 | 2 | 0.72 | 0.68 | 0.69 | $H_2O$ |
| | Ratio (Ext_45Rat) | 3 | 0.07 | -0.05 | -0.17 | 1 | 0.01 | -0.08 | -0.10 | All indices |
| | Ratio max (Ext_45RatMax) | 3 | 0.49 | 0.42 | 0.52 | 2 | 0.44 | 0.37 | 0.39 | All indices |
| Extensograph 90 min | Energy ($cm^2$) (Ext_90En) | 3 | 0.85 | 0.83 | 0.86 | 2 | 0.79 | 0.76 | 0.84 | All indices |
| | Resistance to extension (BU) (Ext_90Res) | 2 | 0.69 | 0.66 | 0.74 | 2 | 0.62 | 0.58 | 0.66 | $H_2O$ |
| | Extensibility (mm) (Ext_90Ext) | 3 | 0.66 | 0.62 | 0.66 | 2 | 0.63 | 0.59 | 0.65 | All indices |
| | Max resistance to extension (BU) (Ext_90Max) | 3 | 0.84 | 0.81 | 0.87 | 2 | 0.77 | 0.75 | 0.83 | All indices |
| | Ratio (Ext_90Rat) | 1 | 0.14 | 0.07 | 0.17 | 1 | 0.12 | 0.05 | 0.08 | $H_2O$ |
| | Ratio max (Ext_90RatMax) | 2 | 0.65 | 0.61 | 0.72 | 2 | 0.60 | 0.55 | 0.65 | $H_2O$ |
| Extensograph 135 min | Energy ($cm^2$) (Ext_135En) | 3 | 0.84 | 0.82 | 0.87 | 2 | 0.79 | 0.77 | 0.87 | All indices |
| | Resistance to extension (BU) (Ext_135Res) | 3 | 0.78 | 0.75 | 0.60 | 2 | 0.69 | 0.67 | 0.62 | NaCl |
| | Extensibility (mm) (Ext_135Ext) | 2 | 0.60 | 0.56 | 0.64 | 2 | 0.60 | 0.56 | 0.61 | $H_2O$ |
| | Max resistance to extension (BU) (Ext_135Max) | 3 | 0.87 | 0.86 | 0.76 | 2 | 0.80 | 0.78 | 0.76 | All indices |
| | Ratio (Ext_135Rat) | 2 | 0.43 | 0.37 | 0.36 | 1 | 0.33 | 0.28 | 0.31 | $H_2O$ |
| | Ratio max (Ext_135RatMax) | 2 | 0.79 | 0.77 | 0.84 | 2 | 0.69 | 0.66 | 0.81 | All indices |

**Figure 1**

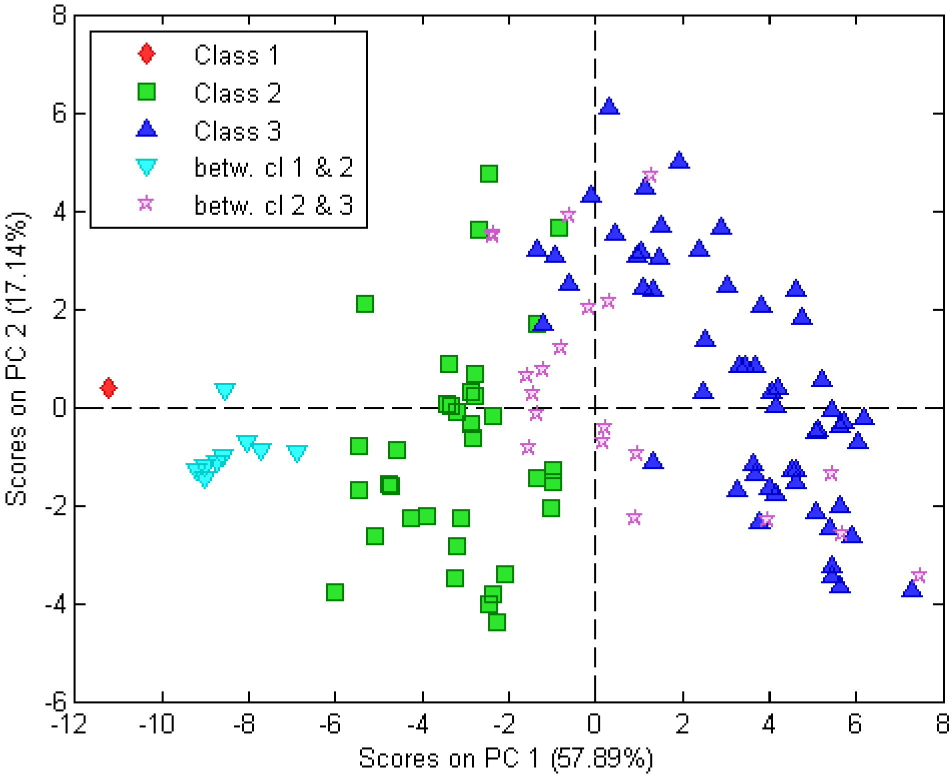

Class 1
Class 2
Class 3
betw. cl 1 & 2
betw. cl 2 & 3
Scores on PC 2 (17.14%)
Scores on PC 1 (57.89%)
8
6
4
2
0
-2
-4
-6
-12
-10
-8
-6
-4
-2
0
2
4
6
8

**Figure 2**

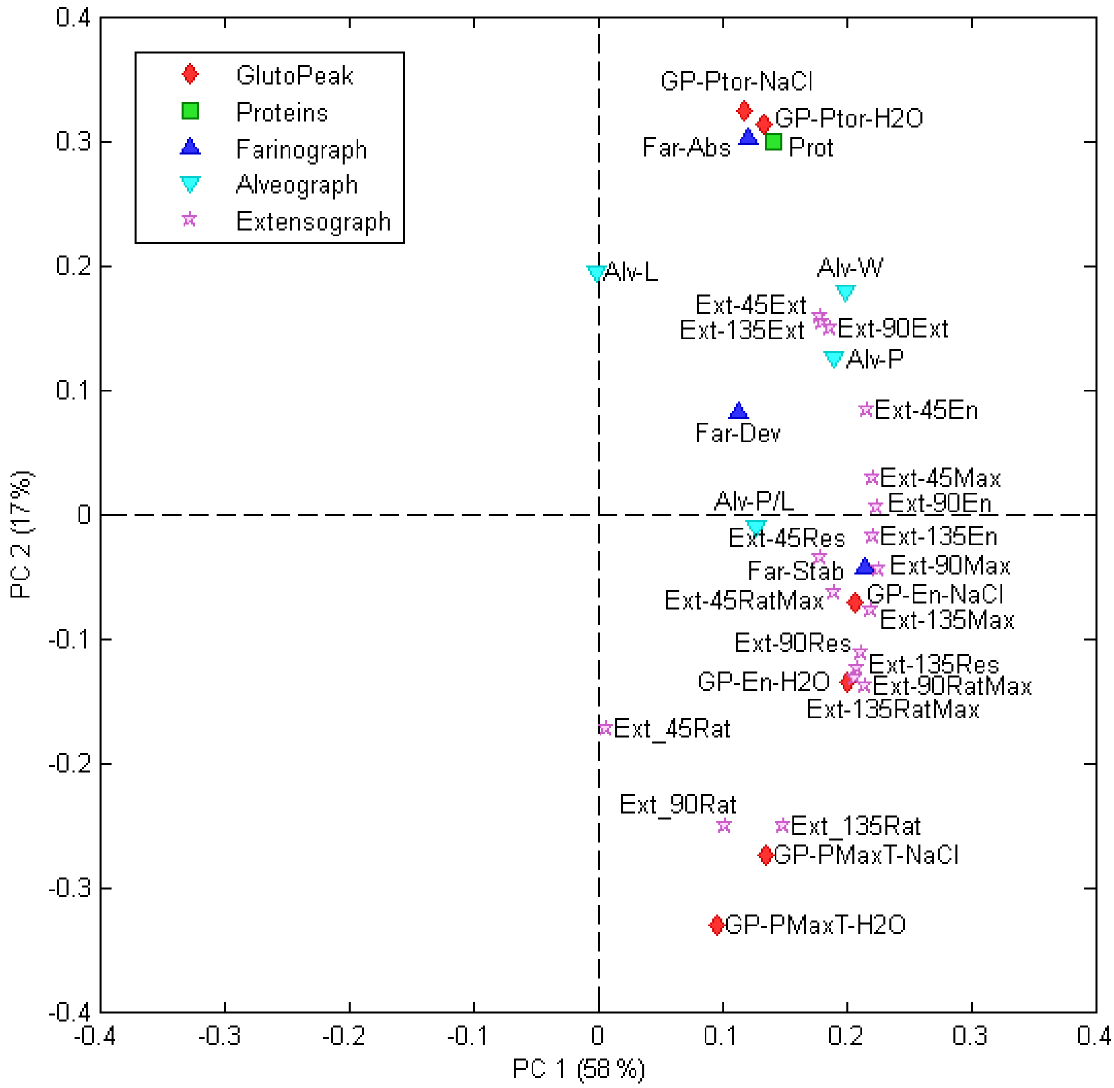
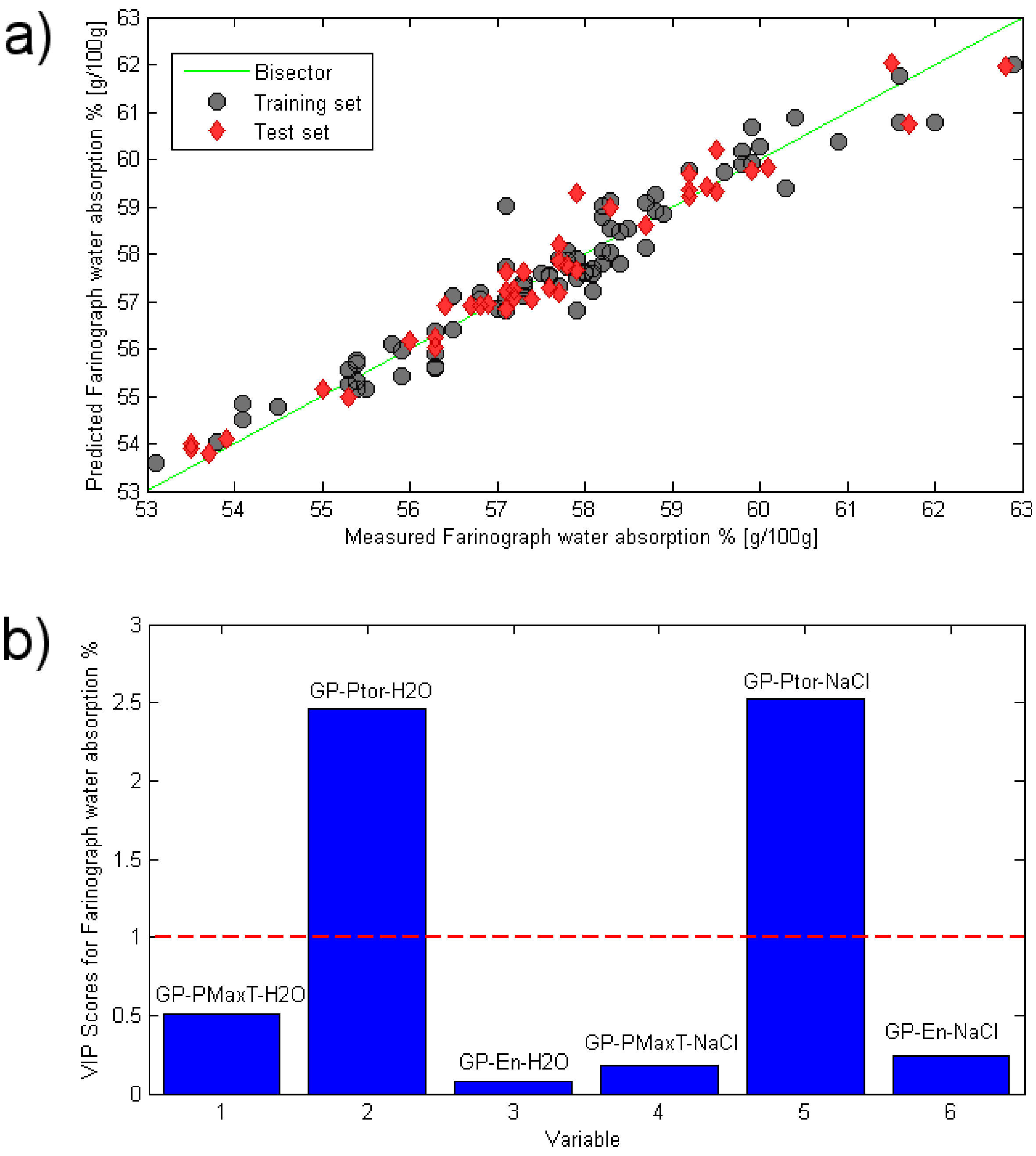
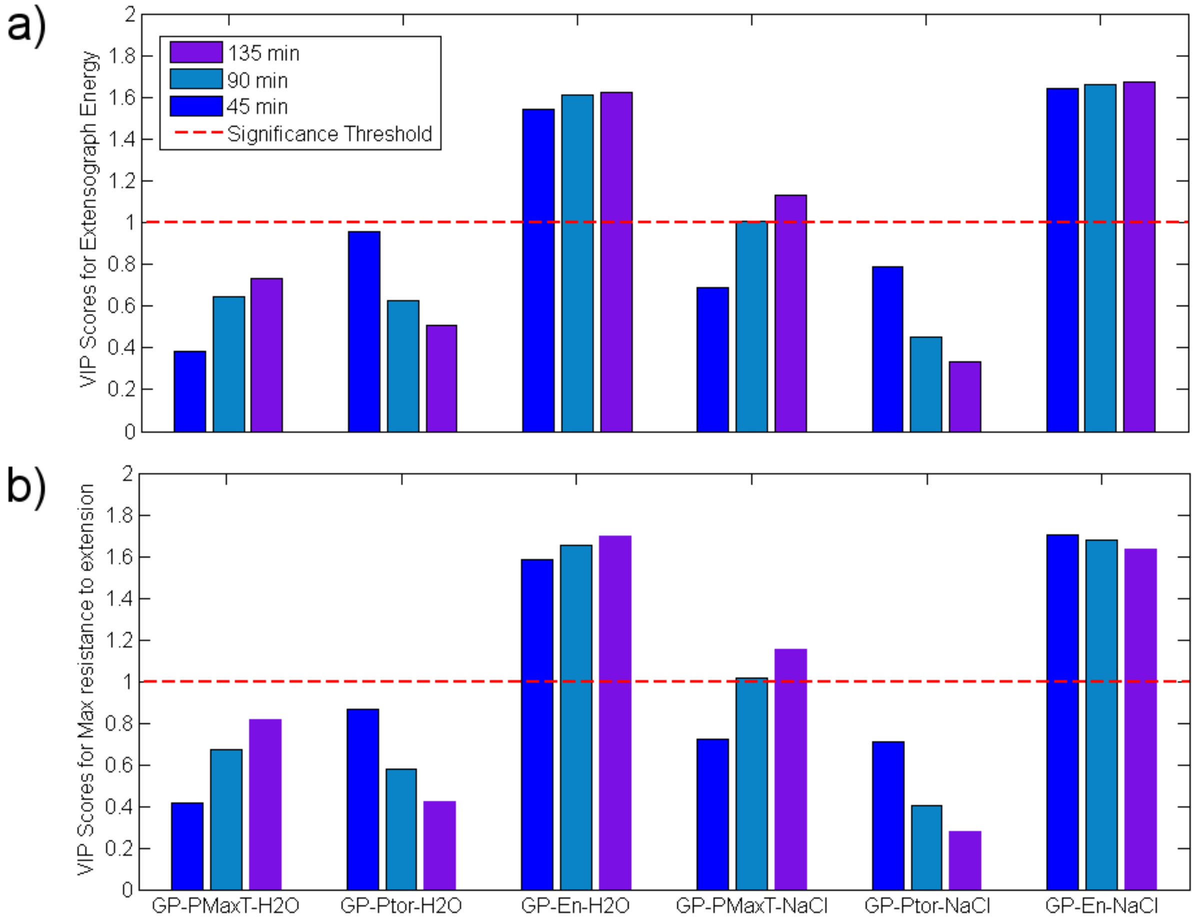

GlutoPeak
Proteins
Farinograph
Alveograph
Extensograph
GP-Ptor-NaCl
GP-Ptor-H2O
Far-Abs
Prot
Alv-L
Alv-W
Ext-45Ext
Ext-135Ext
Ext-90Ext
Alv-P
Ext-45En
Far-Dev
Ext-45Max
Alv-P/L
Ext-90En
Ext-45Res
Ext-135En
Far-Stab
Ext-90Max
Ext-45RatMax
GP-En-NaCl
Ext-135Max
Ext-90Res
Ext-135Res
GP-En-H2O
Ext-90RatMax
Ext-135RatMax
Ext_45Rat
Ext_90Rat
Ext_135Rat
GP-PMaxT-NaCl
GP-PMaxT-H2O
PC 1 (58 %)
PC 2 (17%)
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4

**Figure 3**



a)
Bisector
Training set
Test set
Predicted Farinograph water absorption % [g/100g]
Measured Farinograph water absorption % [g/100g]
53
54
55
56
57
58
59
60
61
62
63
b)
VIP Scores for Farinograph water absorption %
Variable
GP-PMaxT-H2O
GP-Ptor-H2O
GP-En-H2O
GP-PMaxT-NaCl
GP-Ptor-NaCl
GP-En-NaCl
0
0.5
1
1.5
2
2.5
3
1
2
3
4
5
6

**Figure 4**


a)
b)
VIP Scores for Extensograph Energy
VIP Scores for Max resistance to extension
135 min
90 min
45 min
Significance Threshold
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
GP-PMaxT-H2O
GP-Ptor-H2O
GP-En-H2O
GP-PMaxT-NaCl
GP-Ptor-NaCl
GP-En-NaCl