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1 **CHARACTERIZATION OF COMMON WHEAT FLOURS (*TRITICUM AESTIVUM L.*)**

2 **THROUGH MULTIVARIATE ANALYSIS OF CONVENTIONAL RHEOLOGICAL**

3 **PARAMETERS AND GLUTEN PEAK TEST INDICES**

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13 **ABSTRACT**

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

28

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

31

32 **Abbreviations:** Alv-W, Alveographic strength; Alv-P, Alveographic tenacity, Alv-L, Alveographic
33 extensibility; Alv-P/L, Alveographic tenacity; AU, Arbitrary Unit; BE, Brabender Equivalent;
34 Ext_45En, Extensographic energy (45 min); Ext_90En, Extensographic energy (90 min);
35 Ext_135En, Extensographic energy (135 min); Ext_45Ext, Extensographic extensibility (45 min);
36 Ext_90Ext, Extensographic extensibility (90 min); Ext_135Ext, Extensographic extensibility (135
37 min); Ext_45Max, Extensographic maximal resistance to extension (45 min); Ext_90Max,
38 Extensographic maximal resistance to extension (90 min); Ext_135Max, Extensographic maximal

39 resistance to extension (135 min); Ext_45Rat, Extensographic Ratio (45 min); Ext_90Rat,
40 Extensographic Ratio (90 min); Ext_135Rat, Extensographic Ratio (135 min); Ext_45RatMax,
41 Extensographic Ratio Max (45 min); Ext_90RatMax, Extensographic Ratio Max (90 min);
42 Ext_135RatMax, Extensographic Ratio Max (135 min); Ext_45Res, Extensographic resistance to
43 extension (50 mm; 45 min); Ext_90Res Extensographic resistance to extension (50 mm; 90 min);
44 Ext_135Res, Extensographic resistance to extension (50 mm; 135 min); Far-Abs, Farinographic
45 Water Absorption; Far-Dev, Farinographic Dough development time; Far-Stab, Farinographic
46 Stability; FN, False Negative; FP, False Positive; FU, Farinograph Unit; LV, Latent Variables; GP-
47 En, GlutoPeak Energy; GP-PmaxT, GlutoPeak Peak Maximum Time; GP-Ptor, GlutoPeak
48 Maximum Torque; PCA, Principal Component Analysis; PLSR, Partial Least Squares Regression;
49 Prot, protein content; R^2_{CAL} , squared correlation coefficient referred to the calibration of the training
50 set; R^2_{CV} , squared correlation coefficient in Cross-Validation; R^2_{PRED} , squared correlation
51 coefficient for the prediction of the external test set; RMSE, Root Mean Square Error; RMSEC,
52 Root Mean Square Error in Calibration of the training set; RMSECV, Root Mean Square Error in
53 Cross-Validation; RMSEP, Root Mean Square Error in Prediction of the external test set; TN, True
54 Negative; TP, True Positive; VIP, Variable Importance in Projection.

55

56 **1. Introduction**

57 Common wheat (*Triticum aestivum L.*) is used in a wide range of applications ranging from bread,
58 pastries, biscuits and cakes to noodles and pasta. The functionality and versatility of flour is
59 associated with the capacity of its storage proteins - gliadins and glutenins - to form gluten.
60 Although each wheat flour can organize its storage proteins into a viscoelastic network, its
61 characteristics can greatly differ according to genotype and environmental conditions (Gupta,
62 Batey, & MacRitchie, 1992; Hasniza, Wilkes, Uthayakumaran, & Copeland, 2014). Therefore,
63 different classes of wheat are suited for different types of products to deliver certain functional
64 attributes. For example, flours from strong wheat varieties are preferred for bread where a strong
65 gluten network is desired. On the other hand, soft wheat is preferred for cookies and cakes, where a
66 weak gluten network is desirable. The technological behavior of flour is not only linked to the
67 protein and gluten content, but it is also the result of complex interactions between macromolecules
68 that are responsible for dough performances. Consequently, flour classification is expressed by
69 several parameters, usually measured by rheological approaches that generally provide a
70 quantitative description of mechanical properties (Dobraszczyk & Morgenstern 2003). Attempts to
71 describe the physical properties of doughs have resulted in the design of many rheological devices.
72 Some of these instruments were designed to determine, for instance, the amount of mixing that
73 dough requires or the amount of water that should be added to the flour to obtain dough of the
74 desired consistency (e.g. Farinograph by Brabender®). Others simulate the rounding, and molding
75 in the baking process and measure the dough resistance to uniaxial extension (Extensograph by
76 Brabender®) or to the 3-D extension (Alveograph by Chopin Technologies), in order to determine
77 the dough strength properties useful for predicting bread-making quality. Finally, the Mixolab by
78 Chopin Technologies is a quite new instrument used to characterize the rheological behavior of
79 dough subjected to the simultaneous action of mixing and temperature (Dubat, 2013). The
80 rheological tests - currently used in research laboratories and companies operating in the sector -
81 together with their points of strength and weaknesses, are summarized in Table 1. Although the

82 rheological properties of wheat are considered of great importance for determining baking quality
83 and useful tools for predicting process efficiency (e.g. dough yield, leavening conditions, and so on)
84 and product quality (e.g specific volume, textural attributes) (Olivier & Allen, 1992; Dowell et al.,
85 2008; Mondal & Datta 2008; Ktenioudaki, Butler, & Gallagher, 2010; Banu, Stoenescu, Ionescu, &
86 Aprodu, 2011), most of the procedures are time consuming and require a large amount of samples.
87 The GlutoPeak has been recently proposed for the evaluation of wheat flour quality by measuring
88 the aggregation behaviour of gluten (Kaur Chandi & Seetharaman, 2012). The test has been also
89 proposed as a valid screening tool for durum wheat quality (Mart, Seetharaman, & Pagani, 2013;
90 Marti, Cecchini, D'Egidio, Dreisoerner, & Pagani, 2014). The GlutoPeak indices were significantly
91 correlated with the conventional parameters used for durum wheat characterization and pasta-
92 quality prediction, with the advantages of requiring few minutes of analysis (5-10 minutes) and
93 small amount of sample (9 g). These characteristics are of great interest not only in the durum value
94 chain but also in common wheat sector, and especially in breeding programs. During the test, the
95 sample is mixed with water (flour : water ratio equal to 0.9 : 1) and subjected to intense mechanical
96 action, due to the high speed of the rotating element (set at a constant value between 1900 and 3000
97 rpm). These conditions - allowing for the formation of the gluten network- initially promote a
98 strong increase in the consistency of the slurry, until reaching a maximum value. Then, the
99 continuous mechanical stress causes the breakdown of the gluten network, which is recorded as a
100 decrease in consistency.

101 In this study, a large number of wheat flour samples - characterized by different end-uses -
102 was analyzed both considering the chemical and rheological indices conventionally used in the
103 cereal chain (protein content and Farinograph, Alveograph and Extensograph parameters) and the
104 indices derived from the new GlutoPeak test. In order to investigate the correlations existing
105 between the conventional rheological parameters and the GlutoPeak indices, a multivariate
106 statistics-based approach was used, consisting in a data exploration step through Principal
107 Component Analysis (PCA) (Cocchi et al., 2004; Bro & Smilde, 2014), followed by the

108 development of multivariate calibration models using Partial Least Squares Regression (PLSR)
109 (Wold, Sjöström, & Eriksson, 2001; Foca, Masino, Antonelli, & Ulrici, 2011). Moreover, the
110 possibility of using the GlutoPeak indices for the assessment of the wheat flour quality category
111 was also investigated, through the comparison between the class assignments made by the miller on
112 the basis of the Alveograph W values and the corresponding assignments made using the W values
113 predicted by the PLSR model.

114

115 **2. Materials and Methods**

116 **2.1. Materials**

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

121

122 **2.2 Empiric rheological tests**

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

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

134 30.02, 2000). The following indices were considered: *i*) P or tenacity (mm H₂O) - corresponding to
135 the maximum pressure on deformation; *ii*) L or extensibility (mm) - corresponding to the length of
136 the curve; *iii*) W or strength (*10⁻⁴ J) - corresponding to the area under the curve; *iv*) P/L ratio.

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

145

146 **2.3 GlutoPeak Test**

147 The gluten aggregation properties of flours were measured using the GlutoPeak (Brabender GmbH
148 and Co KG, Duisburg, Germany). An aliquot of 9 g of flour was dispersed in 10 ml of solvent. Both
149 double distilled water (H₂O) and 0.33 M Sodium Chloride (NaCl) solution were considered, in
150 order to evaluate the possible differences between the results obtained using these two different
151 solvents. In particular, the tests with NaCl were carried out to mimic the conditions used with the
152 Extensograph measurements, which involved the addition of 2 g / 100 g NaCl. Sample and solvent
153 temperature was maintained at 35 °C by circulating water through the jacketed sample cup. The
154 paddle was set to rotate at 3000 rpm and each test was run for 10 min. The main indices
155 automatically evaluated by the software provided with the instrument (Brabender GlutoPeak
156 v.1.1.0) are: *i*) Maximum Torque expressed in Brabender Equivalentents (BE) - corresponding to the
157 peak occurring as gluten aggregates; *ii*) Peak Maximum Time expressed in seconds - corresponding
158 to the time at peak torque. In addition, the area under the peak - expressed in arbitrary units (AU)
159 and corresponding to the energy required for gluten aggregation was calculated using Microsoft

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

162

163 **2.4 Definition of the wheat flour quality classes**

164 With particular regards to the leavened baked goods, two main categories can be identified as
165 chemical and biological leavening. The latter can be further distinguished according to the method
166 used for the leavening phase: the straight-dough and the sponge-and-dough processes (Pagani,
167 Lucisano, & Mariotti, 2014). In particular, in Italy about 15% of the wheat flour production is
168 dedicated to the preparation of chemically and physically leavened products such as biscuits and
169 cakes, while 70% is addressed to the production of biologically leavened goods such as bread and
170 pizza (www.infofarine.it). Generally, mill companies are used to prepare suitable wheat kernel
171 mixtures in order to obtain flours that satisfy customers' needs. To this aim, the W alveographic
172 index – which is related to flour strength - is generally considered to define the technological
173 behavior of flours. According to this criterion, three types of common wheat flours are in fact
174 identified by the miller (Molino Quaglia S.p.A.) as follows: i) *class 1*: chemically leavened
175 products ($100 * 10^{-4} \text{ J} < W < 130 * 10^{-4} \text{ J}$); ii) *class 2*: straight-dough systems ($180 * 10^{-4} \text{ J} < W < 280$
176 $* 10^{-4} \text{ J}$); iii) *class 3*: sponge-and-dough systems ($W \geq 320 * 10^{-4} \text{ J}$).

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

186

187 **2.5 Data Analysis**

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

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

196 Then, for the calculation of the PLSR calibration models, the whole dataset was split into a
197 dataset X with size $\{120 \times 6\}$, containing the GlutoPeak indices, and a dataset Y with size $\{120 \times$
198 $26\}$, composed by the remainder parameters. Each single parameter determined with the
199 conventional methods (y_i variable corresponding to the i -th column of dataset Y) was considered
200 separately as a dependent variable for the construction of the calibration models. For each y
201 variable, the PLSR models were calculated considering three possible options as for the descriptor
202 variables: all the six GlutoPeak indices, only the three Glutopeak indices measured using water as
203 solvent, and only the three Glutopeak indices measured using the NaCl aqueous solution as solvent.
204 Notwithstanding the very low number of descriptor variables, PLSR was used instead of Multiple
205 Linear Regression (MLR) due to the presence of correlated variables within the X block. Both the
206 X and Y datasets were randomly split into a training set, containing 80 samples (i.e., $2/3$ of the
207 objects of the whole dataset), and a test set, containing the remainder 40 samples, to be used for
208 external validation. X and Y variables were preprocessed by autoscaling, and the optimal number of
209 latent variables (LVs) was chosen by minimizing the error in cross-validation (random group cross-
210 validation, with 10 deletion groups and 20 iterations). The selected model was finally validated by
211 means of the test set.

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

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

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

237 incorrectly classified as positive) and False Negative rate (FN, i.e., proportion of positive cases that
238 were incorrectly classified as negative).

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

242

243 **3. Results and Discussion**

244 **3.1 PCA on the whole dataset**

245 The structure of the whole dataset was explored by means of PCA: a 2 Principal Components (2
246 PCs) model was obtained, explaining 75% of the whole data variance. The PC1 vs. PC2 score plot
247 is reported in Fig. 1, showing that the wheat flour quality classes are mainly separated along PC1,
248 which accounts by itself for 58% of data variance. In particular, the only sample belonging to class
249 1 is positioned at the lower value of PC1 and is quite well separated from the “between class 1 and
250 2” samples, which in turn form a quite compact cluster, adjacent to the cluster of class 2 samples.
251 These latter ones are instead partially superimposed to the samples belonging to class 3, and the
252 “between class 2 and 3” samples lie as expected between the respective upper and lower classes,
253 with a quite high degree of superimposition. The gradual variation of the positions of samples with
254 increasing quality class and the partial superimposition of the classes is not surprising, since wheat
255 flour quality is a complex property that varies in a continuous manner and actually relies on several
256 physical, chemical and rheological characteristics, so that the univocal and certain attribution of a
257 given sample to a quality class is not straightforward at all, and the definition of “wheat quality
258 class” by itself is still a debated problem (Foca et al., 2007). This consideration is confirmed by the
259 corresponding loading plot, reported in Fig. 2, which shows that almost all the variables contribute
260 significantly to PC1, with positive values. This means that in general flour wheat strength is
261 correlated with increasing values of almost all the measured parameters. A further differentiation
262 among the analyzed samples is observed along PC2 (17% explained variance), and can be mainly

263 ascribed to two groups of variables. The former one, at positive values of PC2, corresponds to
264 Farinograph water absorption (Far-Abs), protein content (Prot), and GlutoPeak maximum torque
265 expressed in Brabender Equivalents measured both using water and NaCl solution (GP-Ptor-H₂O
266 and GP-Ptor-NaCl, respectively). The second group of variables, at negative values of PC2, is
267 composed by the GlutoPeak peak maximum time (GP-MaxT-NaCl and GP-MaxT-H₂O for
268 measurements made with water or NaCl solution, respectively), and by the Extensograph ratio
269 between extensibility and resistance measured after 90 and 135 min (Ext_90Rat and Ext_135Rat,
270 respectively). Interestingly, GlutoPeak indices contribute significantly both to PC1 (mainly as for
271 the area under the peak, i.e., GP-En-NaCl and GP-En-H₂O), and to PC2.

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

275

276 **3.2 PLSR models**

277 The results of the PLSR calibration models of the 26 reference parameters calculated using all the 6
278 GlutoPeak indices are reported in Table 3 in terms of model dimensionality (i.e., number of selected
279 latent variables, LVs), RMSE and R^2 statistics. On the whole, considering the R^2_{PRED} values,
280 acceptable to good results ($R^2_{\text{PRED}} \geq 0.6$) were obtained for 18 out of the 26 considered parameters.
281 As expected, GlutoPeak indices are well correlated with the total protein content ($R^2_{\text{PRED}} = 0.91$).
282 The values of the GlutoPeak maximum torque expressed in Brabender Equivalents (GP-Ptor-H₂O
283 and GP-Ptor-NaCl) are the only variables with significant VIP score values (equal to 2.5 for both),
284 confirming what was already observed in the loading plot of Fig. 2.

285 The best overall performance was obtained for the prediction of Farinograph water absorption
286 ($R^2_{\text{PRED}} = 0.96$), whose y predicted vs. y experimental plot is reported in Fig. 3a. The value of the
287 Root Mean Square Error in Prediction of the external test set obtained by the PLSR model of Far-
288 Abs (RMSEP = 0.44%, *see* Table 3) is comparable with the value of the average experimental error

289 (equal to 0.24%). This latter value was calculated as the square root of the ANOVA within-sample
290 mean square value, using five replicate experimental measurements made on a subset of flour
291 samples (data not reported for conciseness reasons). The model prediction error and the
292 experimental error values are comparable each other, which can be considered as satisfactory. In
293 fact, this means that GlutoPeak can provide estimates of Farinograph water absorption with an
294 uncertainty that is only slightly higher than the uncertainty of the reference method, and in much
295 shorter times.

296 The VIP score plot reported in Fig. 3b shows that the GlutoPeak indices that essentially contribute
297 to the calibration model of Farinograph water absorption are the same parameters that were selected
298 for total protein content (GP-Ptor-H₂O and GP-Ptor-NaCl, with equal importance) coherently with
299 the PCA results. The correlation between the peak torque (GlutoPeak test) and the water absorption
300 (Farinograph test) can be likely related to the fact that both the indices are strongly associated with
301 the protein content (Holas & Tipples, 1978, Tipples, Meredith, & Holas, 1978).

302 Among the other Farinograph parameters, also stability is well predicted ($R^2_{\text{PRED}} = 0.88$); in
303 this case, based on the VIP score values, the significant variables are GP-En-NaCl (VIP = 1.6) and
304 GP-En-H₂O (VIP = 1.7) and, to a minor extent, GP-PMaxT-NaCl (VIP = 1.2). Flour samples which
305 exhibit great resistance to mechanical stresses - as those exerted during the GlutoPeak test (3000
306 rpm) - will show great stability during mixing under gentle conditions as those occurring in the
307 Farinograph bowl (63 rpm) and for prolonged time.

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

314 Among the Extensograph parameters, for all the three considered measurement times (45, 90
315 and 135 min) satisfactory models have been obtained for Energy and Max resistance to extension.
316 Interestingly, for both these parameters the VIP score values are very similar, and show almost the
317 same variations with the different measurement times, as it is reported in Fig. 4. This is related to
318 the characteristics of the flours analyzed in the present study. According to the farinographic and
319 alveographic indices, most of them are defined as “strong” flours whose extensibility features do
320 not worsen over time (Table 2), in agreement with their end-uses such as processing that requires
321 long fermentation time (straight-dough or sponge-and-dough systems). GP-En-H₂O and GP-En-
322 NaCl play always the major role, but with increasing the measurement time, also GP-PmaxT-NaCl
323 assumes a statistically significant contribution to the calibration models. Quite acceptable
324 performances have been obtained also for Extensibility, considering the high experimental errors
325 that generally affect this parameter (the average error of replicate experimental measurements being
326 equal to about 5 mm). In particular, the best results have been obtained for measurements at 90 and
327 at 135 min. For these points (90 and 135 min) also the calibration models of Resistance to extension
328 and of Ratio max were acceptable. This behavior can be likely explained by the protein
329 polymerisation occurring during resting (Weegels, van de Pijpekamp, Graveland, Hamer, &
330 Schofield, 1996; Borneo & Khan, 1999).

331 Concerning the Alveograph parameters, it was not possible to estimate L ($R^2_{\text{PRED}} = 0.05$) –
332 which is related to dough extensibility - and, consequently, also its derived parameter P/L ($R^2_{\text{PRED}} =$
333 0.32). Conversely, in the evaluation of the performance of the calibration models for W ($R^2_{\text{PRED}} =$
334 0.73) and P ($R^2_{\text{PRED}} = 0.86$) – related to dough strength and tenacity, respectively - it must be
335 noticed that since these rheological parameters are highly operator dependent, they are affected by
336 an experimental error that may be as high as 10% of the mean value (Foca et al., 2007). In view of
337 this fact, the RMSE values obtained for W and P indicate that these models can be considered as
338 quite satisfactory. As far as Alveograph W is concerned, based on the VIP score values, the
339 statistically significant Glutoppeak indices are GP-Ptor_H₂O and GP-Ptor-NaCl (VIP = 1.6 and 1.4,

340 respectively) and GP-En-H₂O and GP-En-NaCl (VIP = 1.1 and 1.4, respectively). The same indices
341 are the significant ones also for Alveograph P, where GP-Ptor_H₂O and GP-Ptor-NaCl (VIP = 1.8
342 and 1.6, respectively) are both more significant than GP-En-H₂O and GP-En-NaCl (VIP = 1.1 and
343 1.3, respectively). The W values obtained by the PLSR model reported in Table 3 were also used to
344 assign the samples to the different quality classes described in Section 2.4, and the quality class
345 assignments of both the training set and the test set objects were compared with the corresponding
346 assignments made by the miller using the original W values. The results of this comparison,
347 reported in Table 4, show that in general the class assignments made using the GlutoPeak indices +
348 PLSR match acceptably those made by the miller (*see* section 2.4); the greatest errors are observed
349 for the “between class 2 and 3” samples, coherently with what previously observed in the score plot
350 of Fig. 1.

351 Finally, concerning the comparison between the two solvents used for the GlutoPeak
352 measurements, Table 5 reports the R² statistics of the PLSR models obtained using only the
353 GlutoPeak indices measured with water and those of the models obtained with the NaCl solution.
354 Moreover, in order to highlight the conditions leading to the overall best performances for each
355 analyzed parameter, the last column of Table 5 reports the indication of the set of GlutoPeak indices
356 that leads to the highest value of R²_{PRED}, considering also the results reported in Table 3 (i.e., with
357 all the six GlutoPeak indices). On the whole, focusing on the 18 parameters leading to at least
358 acceptable models (i.e., with R²_{PRED} ≥ 0.6), for 8 parameters the best results were obtained
359 considering all the six GlutoPeak indices, for other 8 parameters the best results were obtained with
360 the three GlutoPeak indices measured using water as solvent, and only for 2 parameters the best
361 results were obtained using the three Glutopeak indices measured using the NaCl aqueous solution.
362 Considering that the use of all the six indices requires the execution of two subsequent GlutoPeak
363 runs (one with water and one with NaCl solution), and since the differences between the R²_{PRED}
364 values obtained with all the six indices and those obtained using only the three indices measured
365 using water are however small (the highest difference is equal to 0.05 for Farinograph Stability),

366 this comparison suggests that performing a unique GlutoPeak run using water as solvent could be
367 enough to gain at least an acceptable preliminary estimate of the main chemical and rheological
368 parameters used to define wheat flour behavior.

369

370 **4. Conclusions**

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

385

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389

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Captions to Tables and Figures

- 459 **Table 1.** Rheological approaches currently used for flour characterization
- 460 **Table 2.** Basic statistics of the 32 chemical and rheological parameters.
- 461 **Table 3.** Results of the PLSR calibration models of the 26 reference parameters calculated
462 using all the 6 GlutoPeak indices.
- 463 **Table 4.** Class assignments made using the PLSR model of Alveograph W. *Class 1:*
464 chemically leavened products ($100 * 10^{-4} \text{ J} < W < 130 * 10^{-4} \text{ J}$); *Class 2:* straight-dough
465 systems ($180 * 10^{-4} \text{ J} < W < 280 * 10^{-4} \text{ J}$); *Class 3:* sponge-and-dough systems ($W \geq$
466 $320 * 10^{-4} \text{ J}$). For each class, the following statistics are also reported: TP% = true
467 positives, i.e., percentage of correctly identified samples; TN% = true negatives, i.e.,
468 percentage of correctly rejected samples; FP% = false positives; i.e., percentage of
469 incorrectly identified samples; FN% = false negatives, i.e., percentage of incorrectly
470 rejected samples.
- 471 **Table 5.** Comparison between the performances of the PLSR models calculated using all the
472 six GlutoPeak indices ("*all indices*"), only the three GlutoPeak indices measured
473 using water as solvent ("*H₂O*"), and only the three Glutopeak indices measured
474 using the NaCl aqueous solution ("*NaCl*").
- 475
- 476 **Figure 1.** PC1 vs. PC2 score plot of the whole dataset; symbols indicate the different wheat
477 flour quality classes.
- 478 **Figure 2.** PC1 vs. PC2 loading plot of the whole dataset; symbols indicate the different
479 instrumental techniques.
- 480 **Figure 3.** (a) PLSR Predicted vs. experimentally measured values of Farinograph water
481 absorption (g/100g) and (b) corresponding VIP score plot.
- 482 **Figure 4.** VIP scores for Extensograph Energy (upper plot) and Max resistance to extension
483 (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 |

485 * including sample preparation and cleaning

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

487

488

Table 2

| | | Min | Max | Mean* | Median | Standard deviation |
|--------------------------|--|------|-------|-------|--------|--------------------|
| GlutoPeak | Peak Maximum Time (s) - H ₂ O (GP-PmaxT-H ₂ O) | 63.8 | 164.3 | 113.7 | 110.1 | 21.1 |
| | Maximum Torque (BE) - H ₂ O (GP-Ptor-H ₂ O) | 28.6 | 58.6 | 42.5 | 42.3 | 6.6 |
| | Area under the Peak (AU) - H ₂ O(GP-En-H ₂ O) | 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 ₂ O) (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 |

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

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Table 3

| Parameter | | LVs | RMSEC | RMSECV | RMSEP | R²_{CAL} | R²_{CV} | R²_{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 ₂ O) (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 |

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Table 4

| TRAINING SET | | | | | | | | | | | |
|----------------------|---------------|-----------|-----------|-----------|-----------|-----------|-----|------|------|-----|-----|
| Confusion Table | | | | | | | TP% | TN% | FP% | FN% | |
| | predicted as: | | | | | TOTAL | | | | | |
| | class 1 | > 1 & < 2 | class 2 | > 2 & < 3 | class 3 | | | | | | |
| <i>actual class:</i> | 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 | | | | | | | TP% | TN% | FP% | FN% | |
| | predicted as: | | | | | TOTAL | | | | | |
| | class 1 | > 1 & < 2 | class 2 | > 2 & < 3 | class 3 | | | | | | |
| <i>actual class:</i> | 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 | | | | | |

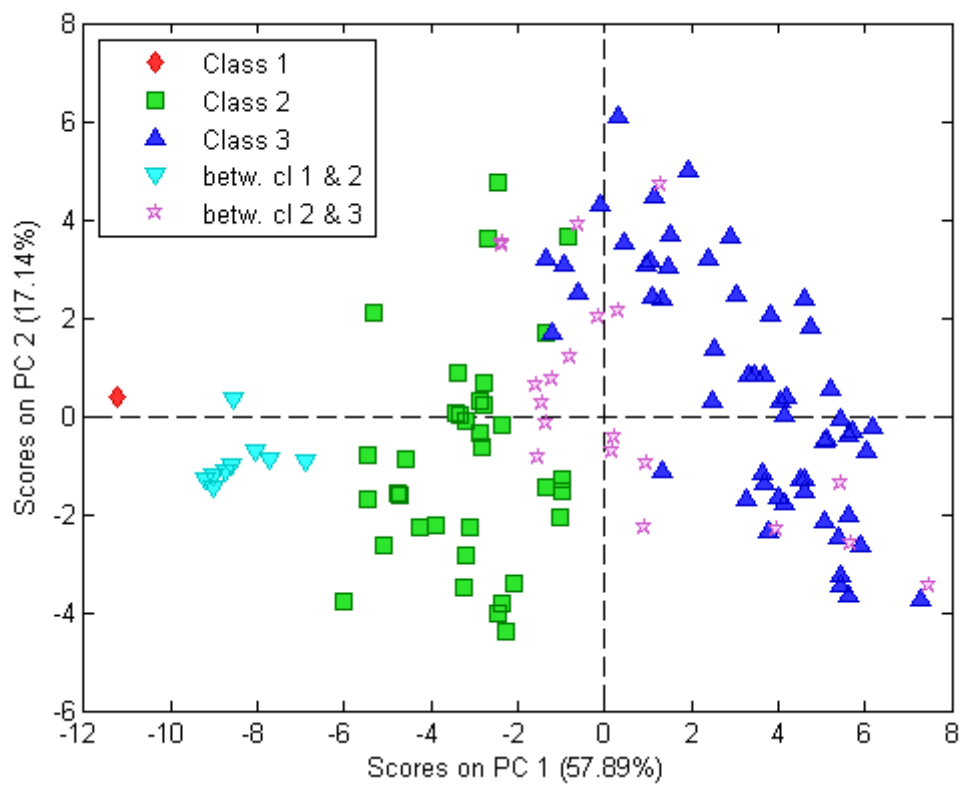
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Table 5

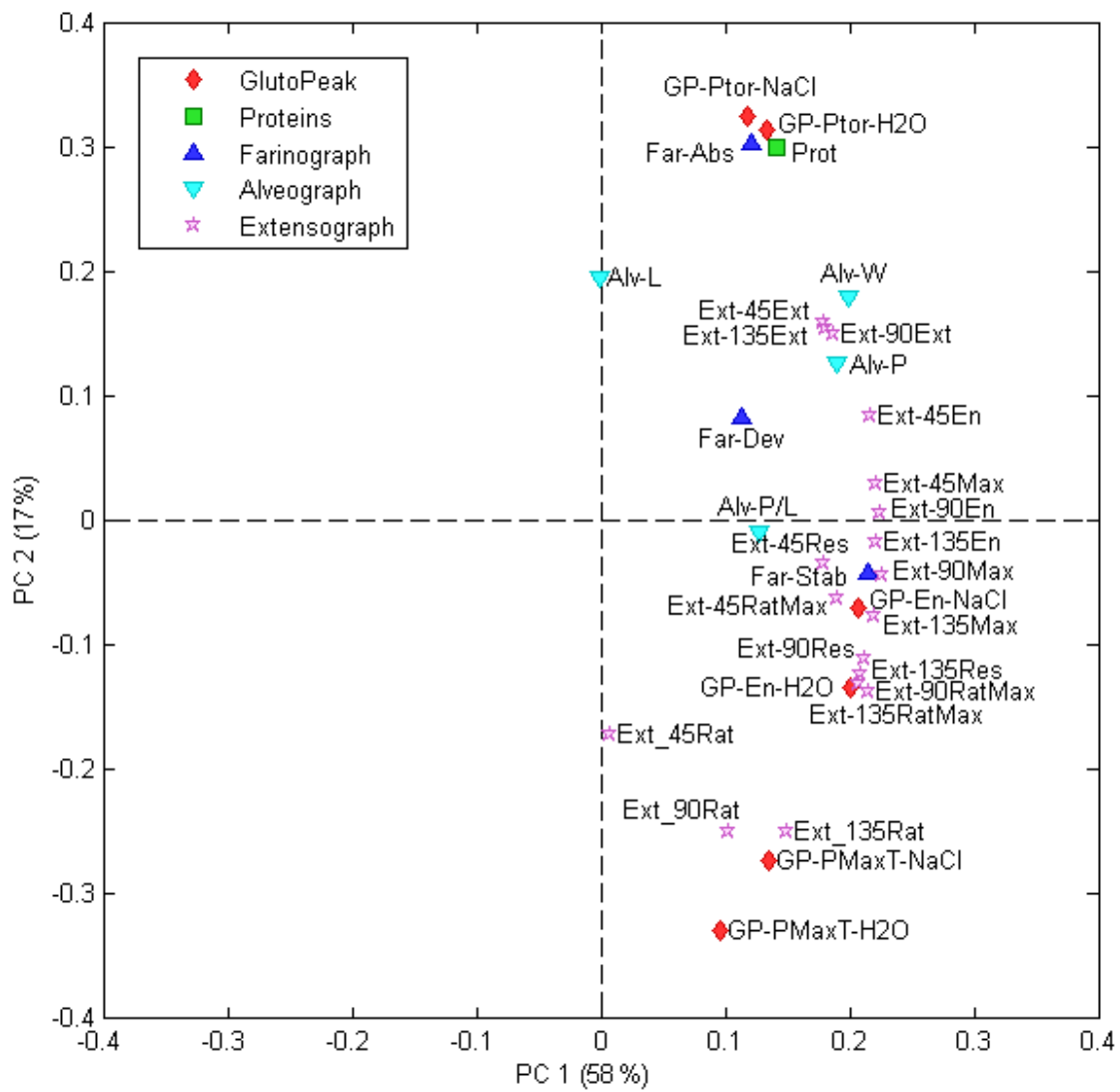
| Parameter | | H ₂ O GlutoPeak indices | | | | NaCl GlutoPeak indices | | | | Best R ² _{PRED} |
|---|---|------------------------------------|-------------------------------|------------------------------|--------------------------------|------------------------|-------------------------------|------------------------------|--------------------------------|-------------------------------------|
| | | 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 |
| Water absorption (%) (Far-Abs) | | 2 | 0.91 | 0.90 | 0.95 | 2 | 0.93 | 0.93 | 0.96 | NaCl |
| Farinograph | 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 ₂ O |
| | P/L (Alv-P/L) | 2 | 0.43 | 0.37 | 0.33 | 2 | 0.42 | 0.35 | 0.31 | H ₂ O |
| | P (mmH ₂ O) (Alv-P) | 3 | 0.82 | 0.80 | 0.87 | 2 | 0.79 | 0.77 | 0.79 | H ₂ O |
| | L (mm) (Alv-L) | 1 | 0.05 | -0.05 | 0.05 | 1 | 0.04 | -0.06 | 0.04 | H ₂ O |
| Energy (cm ²) (Ext_45En) | | 2 | 0.77 | 0.74 | 0.79 | 2 | 0.71 | 0.68 | 0.73 | H ₂ O |
| Resistance to extension (BU) (Ext_45Res) | | 3 | 0.47 | 0.41 | 0.41 | 2 | 0.36 | 0.30 | 0.31 | All indices |
| Extensograph 45 min | Extensibility (mm) (Ext_45Ext) | 2 | 0.59 | 0.55 | 0.64 | 2 | 0.56 | 0.51 | 0.62 | H ₂ O |
| | Max resistance to extension (BU) (Ext_45Max) | 2 | 0.76 | 0.73 | 0.78 | 2 | 0.72 | 0.68 | 0.69 | H ₂ O |
| | 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 |
| | 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 ₂ O |
| Extensograph 90 min | 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 ₂ O |
| | Ratio max (Ext_90RatMax) | 2 | 0.65 | 0.61 | 0.72 | 2 | 0.60 | 0.55 | 0.65 | H ₂ O |
| | 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 |
| Extensograph 135 min | Extensibility (mm) (Ext_135Ext) | 2 | 0.60 | 0.56 | 0.64 | 2 | 0.60 | 0.56 | 0.61 | H ₂ O |
| | 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 ₂ O |
| | Ratio max (Ext_135RatMax) | 2 | 0.79 | 0.77 | 0.84 | 2 | 0.69 | 0.66 | 0.81 | All indices |



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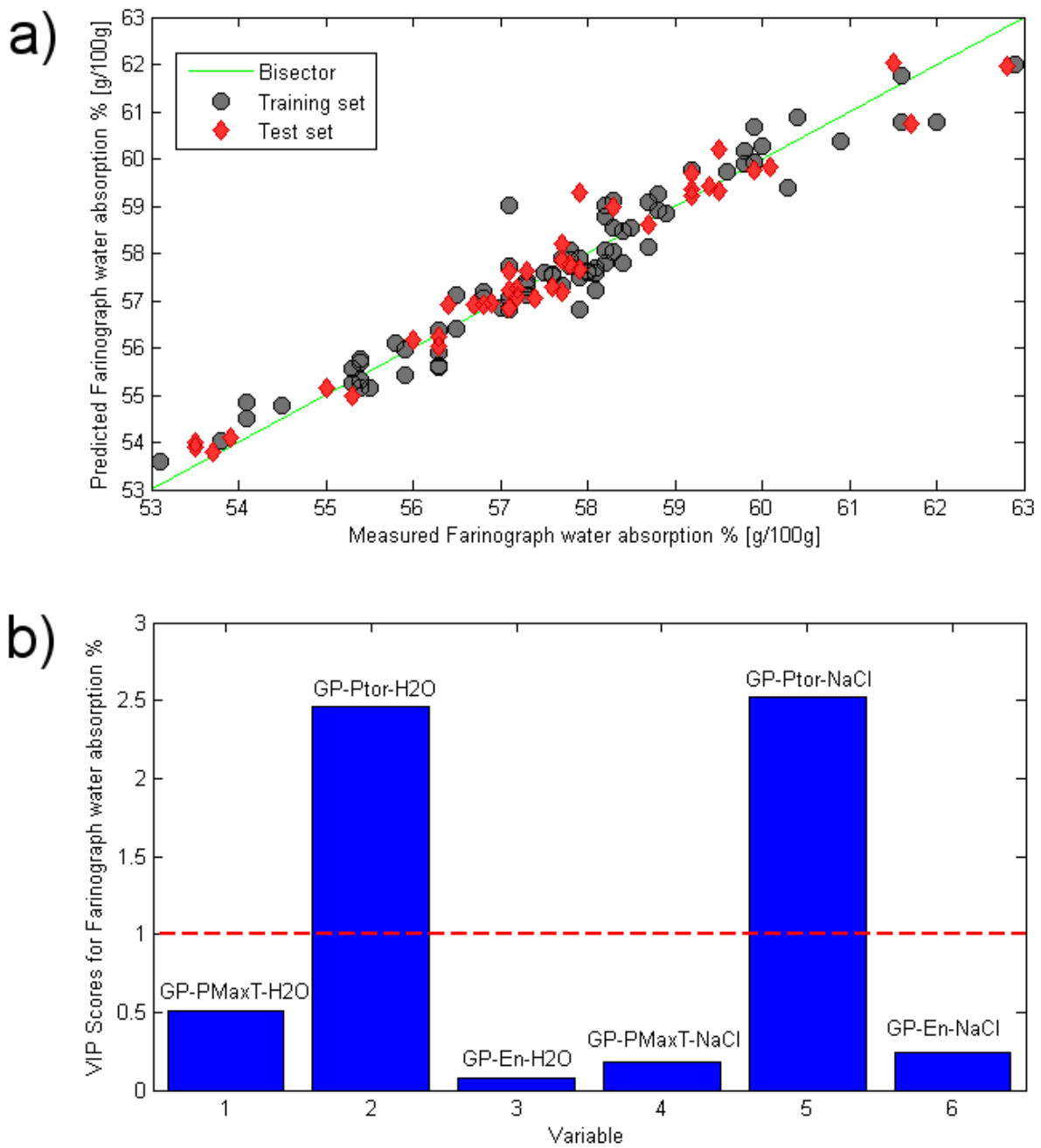
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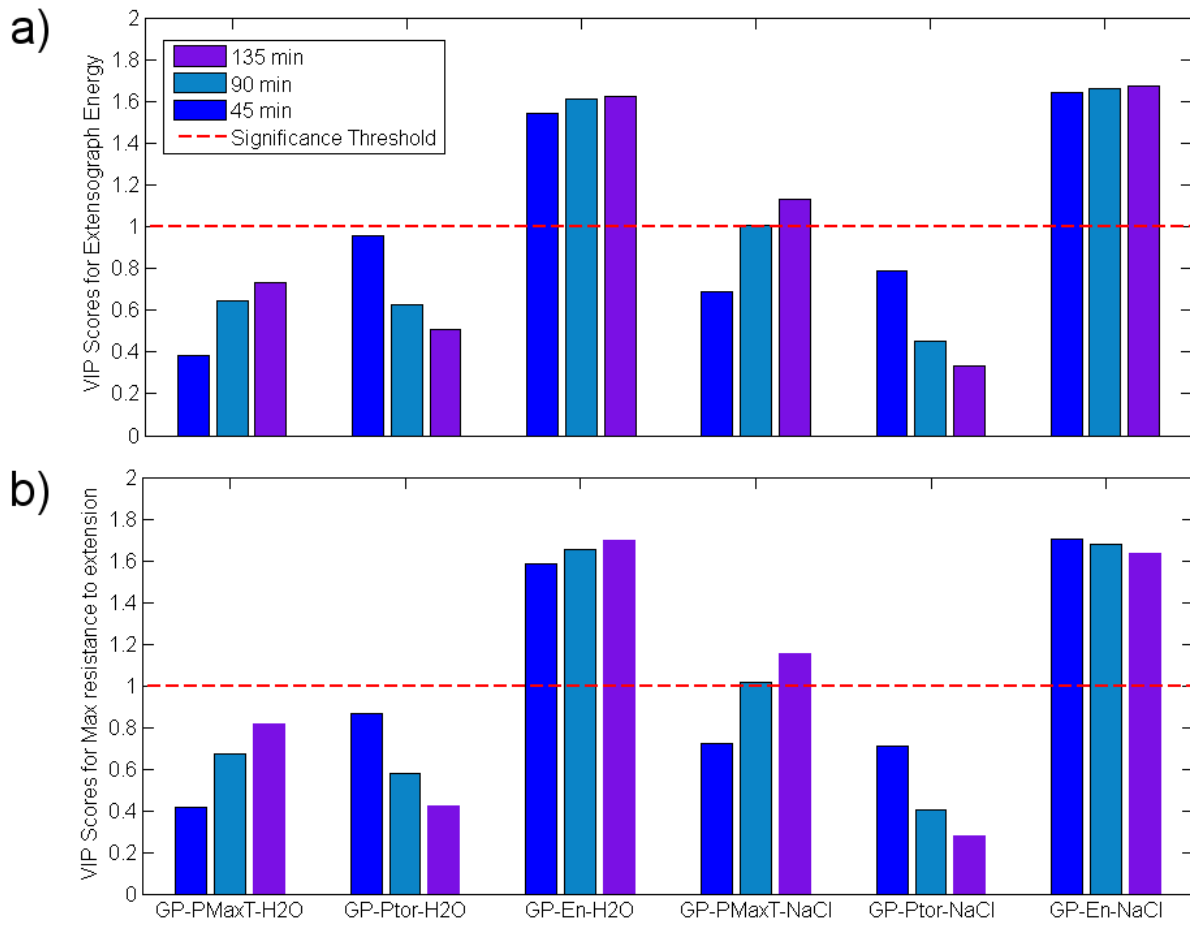
510 **Figure 3**



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513 **Figure 4**



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