Classification of Cereal Flours by Chemometric Analysis of MIR Spectra

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Different kinds of cereal flours submitted to various technological treatments were classified on the basis of their mid-infrared spectra by pattern recognition techniques. Classification in the wavelet domain was achieved by using the wavelet packet transform for efficient pattern recognition (WPTER) algorithm, which allowed singling out the most discriminant spectral regions. Principal component analysis (PCA) on the selected features showed an effective clustering of the analyzed flours. Satisfactory classification models were obtained both on training and test samples. Furthermore, mixtures of varying composition of the studied flours were distributed in the PCA space according to their composition.

KEYWORDS: Cereal flours; infrared spectra; classification; wavelet transform; WPTER; signal processing

INTRODUCTION

The request for rapid, nondestructive, cheap, and accurate methods for food analysis has led to an increasing use of infrared spectroscopy in food analysis (*1, 2*). Fourier transform infrared (FT-IR) spectroscopy, in fact, is a flexible method that can supply qualitative and, in some cases, quantitative information with minimal or no sample preparation. Moreover, it is rapid, sensitive, and relatively low cost (*3*). Since the late 1970s, near infrared (NIR) spectroscopy coupled with chemometrics has been successfully used to characterize cereal samples. Multivariate calibration on NIR spectra is now commonly used for routine analysis to determine protein, moisture, gluten, fiber content, and hardness in flours (*4−6*). Until now, for calibration purposes, the NIR region has been preferred with respect to the medium infrared (MIR) region because of its richness in absorption bands of different intensity bringing the same chemical information. However, recent studies (*7, 8*) have shown that the MIR region can be used to determine the composition of ground cereals with an accuracy equal to or better than that obtained by NIR. MIR competitiveness is to be fundamentally ascribed to the possibility of easier spectra interpretation. The MIR region from 4000 to 400 cm^{-1} is the most widely used range for pure organic compounds identification, but recently the applications of this technique as a nondestructive tool for

characterizing both raw materials and food matrixes composition has been growing.

IR spectroscopy bears information on the chemical composition and physical state of the whole sample, but it is not a selective method. Therefore, to extract useful information from the whole spectra, multivariate data analysis is needed. Different multivariate strategies may be used to accomplish classification tasks on the basis of infrared spectra, but, in general, given the high-dimensionality and the highly correlated nature of the spectral variables, often coupled with a low number of samples, data reduction is almost a mandatory preliminary step. To this aim, two approaches have proven to be successful (*9*): (i) projection of the data onto a smaller subspace, e.g., by principal component analysis (PCA) (*10*); and (ii) selection of the most significant features (*11*). The algorithm employed in this study, namely, the wavelet packet transform for efficient pattern recognition (WPTER) algorithm (*12*), uses both the approaches, decomposing the whole IR spectra into the wavelet packet domain (*13*). There are many advantages when working with wavelet coefficients instead of using the original percent transmittance values in the wavenumber domain. First of all, the continuous nature of the spectral variables is directly taken into account, thus considering both shape and local aspects of the signal. Moreover, the stochastic (noisy) component in the signals is efficiently disjointed by the deterministic (informative) one. In classification tasks, this allows one to derive models that are more robust to spectral noise, and to select contiguous regions of the spectra, which can be more easily interpreted in terms of chemical composition (*12*).

The principal aim of this work is to test the feasibility of using infrared spectra in the MIR region, to discriminate among

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flour samples of different cereals and pseudocereals, namely, wheat, oats, and buckwheat, subjected to different technological treatments, i.e., dehulling, toasting, and puffing. The use of oats and buckwheat is currently limited to the production of low-diffusion or niche foods. When compared to major cereals, such as wheat, maize, and rice, these minor cereals are interesting for their content of natural nutrients and biologically active components. In fact, oats and buckwheat (a dicotyledonous crop traditionally considered a cereal for the structural and chemical features of seed) are rich in fiber and antioxidants, with positive effects on the lipid and carbohydrate metabolism. These two minor cereals also contain lysine-rich proteins, resulting in a biological value similar to that of animal proteins. In the case of oats, the lipid fraction is rich in unsaturated fatty acids. Only limited information is available about the nutritional characteristics and the functional/structural properties of the main macromolecules in these cereals, in particular for what constitutes the protein and the polysaccharide fractions (*14*). For these reasons, we were interested in obtaining information on the spectral regions that are responsible for classification.

Spectra were obtained in transmission mode, after inclusion of a constant amount of flour sample in KBr pellets. PCA was then used on the acquired spectra for explorative investigation, and subsequently the WPTER algorithm was applied, to obtain quantitative classification models and to locate the most discriminant spectral regions. As it was already noted, this is a preliminary study, our long-term interest being the characterization of the technological properties of mixtures obtained by blending the different kinds of flours, by using the same methodological approach. A first step in this direction has been made, by acquiring MIR spectra of wheat flour-based mixtures containing increasing percentages of each of the other studied flours, and analyzing the projection of these mixtures in the space spanned by the principal components (PCs), calculated by using the features selected according to the pure flours classification model.

MATERIALS AND METHODS

Instrumentation. All spectra were collected in transmission mode by using a Bruker IFS 113v FT-IR spectrometer, operating in the region $4000-500$ cm^{-1}, equipped with a sample wheel for the KBr pellets and a TGS pyroelectric detector. All spectral measurements were made at nominal 2 cm^{-1} resolution, with 32 interferograms co-added, zero-filled to double the number of data points and then apodized with a Blackmann-Harris three-term function before Fourier transformation. The single-beam spectra of the samples were divided by single-beam spectra of potassium bromide (reference) to yield transmission spectra.

Samples. Six pure flours of different cereals, namely, wheat, oats, and buckwheat, subjected to different technological treatments, i.e., dehulling, toasting, and puffing, and 10 binary mixtures obtained by blending the wheat flour with each of the other flours in varying proportions, have been analyzed. Various heat-treatments were applied to oats and buckwheat, to inactivate lipid-degrading enzymes, to develop desirable flavors and to induce modifications to the native starch structure that could be useful for product texturization. The toasting treatment consisted of two following steps: a first treatment at 120 °C for 2 h 30 min, and a second one at $1.3-1.4$ atm and $110-115$ °C for 30 min. Then, the obtained toasted cereals were flaked, dried, and cooled. The puffing treatment consisted of a drying step, to bring the cereal at $6-8\%$ final humidity values and, subsequently, of a treatment performed in an expansion room at $9-15$ atm and $200-220$ °C for $30-80$ s. The description of the technological treatments applied to the samples used, together with their codes, is reported in **Table 1**.

The pellets preparation procedure was optimized to obtain as much as possible reproducible spectra, in terms of their superimposition. Although this procedure is more laborious and time-consuming, analysis

Table 1. List of the Sample Codes and Relative Descriptions

code	sample
WF	wheat flour
OF	dehulled oats flour
TOF	dehulled and toasted oats flour
POF	dehulled and puffed oats flour
BF	dehulled buckwheat flour
PBF	dehulled and puffed buckwheat flour
MIX1	20% OF + 80% WF
MIX2	40% OF + 60% WF
MIX3	20% TOF + 80% WF
MIX4	40% TOF + 60% WF
MIX5	20% POF + 80% WF
MIX6	40% POF + 60% WF
MIX7	20% BF + 80% WF
MIX8	40% BF + 60% WF
MIX9	20% PBF + 80% WF
MIX10	40% PBF + 60% WF

time is still reasonable, and we achieved good intra- and interdays reproducibility. Other sample preparation techniques and measuring devices, such as DRIFT (*1*, *2*), may be more advantageous, but this study was essentially aimed at verifying if the information content of the MIR region could be relevant for classification purposes, and therefore the optimization of the acquisition technique will be object of future work.

To gain the highest homogeneity in terms of particle size distribution, all the flour samples, before inclusion in KBr, were milled with a Fritsch Pulverizette 14 Variable Speed Rotor mill equipped with an 80 μm sieve. To decrease the uncertainty due to the pellets preparation, i.e., the error associated with the weighing procedure, for each flour a blend was prepared by mixing it with potassium bromide, to obtain a quantity 10 times higher than the weight of a single pellet. Then, three pellets for each flour sample were prepared by weighing the corresponding aliquots of blend. To test the reproducibility of the pellets preparation, and to minimize the influence of uncontrolled factors on the spectral variability, each KBr/flour blend from the six pure flours was prepared four times in different days. Therefore, on the whole (3 pellets) × (4 sessions) × (6 flours) = 72 spectra were acquired. Of these, 48 (four for each flour) were assigned to the training set and 24 (four for each flour) to the test set, following a Latin square design. As far as the flour mixtures are concerned, the blend with KBr of each flour mixture was prepared twice in different days, and two pellets were made for each KBr blend, for a total amount of (2 pellets) × (2 sessions) × (10 mixtures) = 40 spectra to be used as an external test set.

The KBr/flour ratio in the pellets was optimized, to achieve good spectra reproducibility. The single pellet weight was 180 mg, and three different amounts of included flour were tested: 0.6, 0.9, and 1.2 mg. The spectra that were obtained showed the best reproducibility in correspondence of the highest amount of flour, as can be seen in **Figure 1**.

Data Pretreatment. Before data analysis, each spectrum was normalized by using the standard normal variate (SNV) procedure (*15*). Before explorative PCA, the SNV normalized signals were mean centered. At variance, in the case of the PCA on the wavelet coefficients selected by WPTER, the data were autoscaled, because of the different nature of the wavelet coefficients belonging to different basis vectors.

WPTER Algorithm. The WPTER algorithm is based on the wavelet packet transform (WPT) (*16*), which is an extension of the discrete wavelet transform (DWT). Wavelet transform theory and its applications to chemistry have been recently reviewed in a dedicated book (*13*), where references to the relevant literature may be found; here only few concepts are briefly illustrated. As far as the WPTER algorithm is concerned, a detailed description may be found in the original article (*12*). In the present article, the WPTER algorithm is only schematically summarized, i.e., not all the available options are described, but only the used ones.

The decomposition of each signal in the WPT domain is obtained by applying two filters, which correspond to a given wavelet: a low-pass filter, which preserves the low-frequency content of the signal in
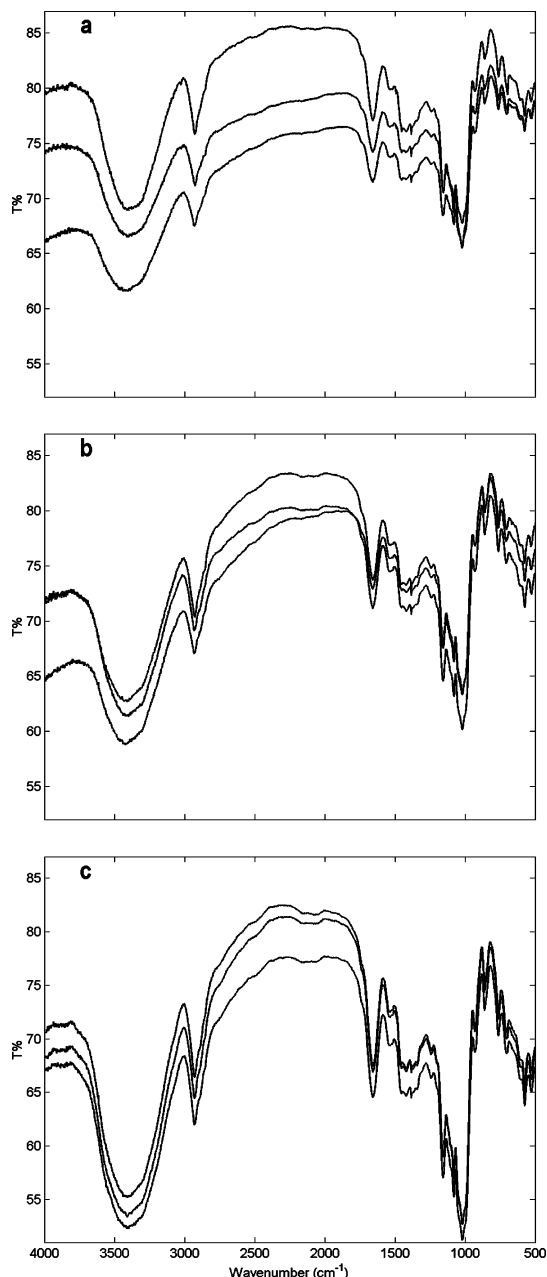
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Figure 1. Spectra of pellets containing different amounts of flour (three replicates for each composition): (a) = 0.6 mg, (b) = 0.9 mg, (c) = 1.2 mg.

the so-called approximations vector, and a high-pass filter, which maintains the high-frequency content in the details vector. This process can be repeated in an iterative way for *j* decomposition levels by applying the two filters both to the approximations and to the details vectors, following a binary tree structure, like in a family tree. Each decomposition level, *j*, is therefore formed by *j* approximations and *j* details vectors, whose length is about halved with respect to the one of the vectors of level *j*−1. The maximum possible decomposition level is the one formed by a number of (approximations + details) vectors corresponding to the power of two, which is equal to or immediately lower than the length of the original signal. This decomposition allows an efficient separation among the different frequencies constituting the original signal, maintaining the local information. It has to be emphasized that a perfect reconstruction of the original signal can be made, by using all the possible combinations of (orthonormal) vectors, in such a way that the whole binary tree is covered horizontally, without any vertical overlap. The first step in WPTER is the WPT decomposition of the signals: given a matrix of size [*m* × *n*] composed by *m*

signals, each one formed by *n* points, a three-dimensional array [*m* × *n* × *j*] called WPMAT is obtained, which contains the projections of all the *m* considered signals into the wavelet packet domain. The level *j* to which arrest the decomposition is chosen by the user. For the reasons given above, WPMAT furnishes a redundant representation of the original signal matrix, since different combinations of vectors, i.e., different bases, can be used for its representation. Therefore, the best basis has to be selected, which in this case is the one leading to the best discrimination among the signals belonging to different classes. Before performing this operation, hard thresholding is made on every approximations and details vector, by retaining only a fixed percentage (user defined) of those wavelet coefficients showing the higher discriminant capability, as evaluated by the between-class/within class variance ratio. Then, the best basis selection is performed in WPTER by using the classification ability (CA) criterion, which is based on the estimation of the Euclidean distance between each couple of objects (signals) in the thresholded wavelet coefficients space. CA is defined as to attain low values in correspondence with the best separation among the objects (spectra) belonging to different classes and, at the same time, the best clustering among the objects belonging to the same class. The best discriminant basis is therefore identified as the one containing the approximations and details vectors attaining the lowest CA values. The basis is not forced to be complete, since the goal is not the perfect signal reconstruction, but the identification of those features, which are important to the classification task.

Once the best classification ability basis (CAB) has been identified, the wavelet coefficients therein contained can be used for signals reconstruction and classification. Each signal is in fact reconstructed back into the original domain by using only the previously selected wavelet coefficients belonging to the CAB and setting to zero the others. These reconstructed signals represent the projection of the selected wavelet coefficients in the original domain, highlighting the signal regions responsible for classification. The classification is then performed using the percentage of assignation (PA), calculated for each one of the reconstructed signals with respect to the mean reconstructed signal of each class. The PA parameter assumes values varying in the 0−100 range, and it is defined according to the following: each one of the *p* nonzero points of a given reconstructed signal lying in the interval given by the value of the corresponding point in the mean reconstructed signal of the considered class ± twice its standard deviation contributes with a value of $1/p$ %. Otherwise, if the considered point does not lie in this interval, its contribution to the corresponding PA value is null. In the ideal event in which every reconstructed signal is assigned in all its points exclusively to the proper class, PA results are equal to 100 for all the signals with respect to their own classes and to 0 for all the signals with respect to the other classes. Obviously, all the intermediate cases are possible. The PA values calculated for each object with respect to each class are represented in a three-dimensional bar graph.

The classification model created on the basis of the training set signals can then be validated by applying it to a set of test signals. Following the same procedure as for the training set, the test set signals are first decomposed into the WPT domain, and then reconstructed back into the original domain, using only the previously selected wavelet coefficients belonging to the CAB. The reconstructed test set signals are then evaluated with respect to the existing classes by using the PA parameter.

Furthermore, for interpretative purposes, for each class the corresponding mean original signal is plotted, highlighting the regions corresponding to the selected features.

To find the optimal classification models, it is possible to vary different parameters, such as the type of wavelet used for the WPT decomposition, the maximum level of decomposition, and the percentage of coefficients retained in the thresholding operation. Therefore, many cycles of calculation, corresponding to all the possible combinations of the different parameters settings have to be performed. For each cycle, the effectiveness of the classification is evaluated by means of a score function (SF) based on the PA parameter. The results are shown in score graphs reporting the SF values of each cycle of calculation, where the most effective classification models are easily identified as those giving the lowest values.
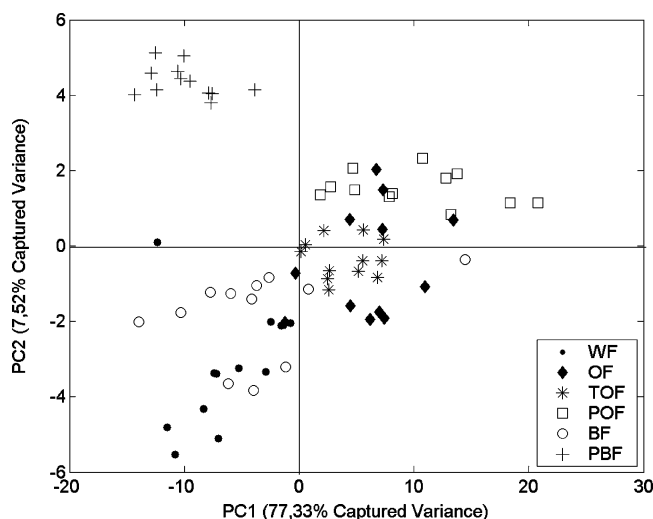
Figure 2. Score plot of the first two PCs obtained by PCA of the MIR spectra of the pure flours. The codes used are those given in **Table 1**.

In the present work, all the combinations resulting from the values of the parameters listed below have been tested, leading to 300 cycles of calculations. Twenty-five wavelets have been used, i.e., 10 daubechies (db1, db2, db3, db4, db5, db6, db7, db8, db9, db10), 5 coiflets (coif1, coif2, coif3, coif4, coif5), 5 symlets (sym4, sym5, sym6, sym7, sym8), 2 biorthogonal wavelets (bior2.4, bior4.4), and 3 reverse biorthogonal wavelets (rbio3.1, rbio3.3, rbio3.9); two values of the maximum decomposition level have been considered (5 and 7), and six percentage values of wavelet coefficients to be retained after thresholding (0.1, 0.5, 1, 3, 5, and 10).

Software. WPTER has been written in MATLAB language and uses some routines from the Wavelet Toolbox 2.1 for MATLAB (*17*). All calculations were carried out using MATLAB 6.5. PCA was run using the PLS Toolbox for MATLAB (*18*).

RESULTS AND DISCUSSION

Explorative PCA of the SNV normalized pure flours spectra shows that the chemical information extracted from the MIR spectra is potentially useful to discriminate the different cereal flours. In fact, the scores plot of the first two PCs, reported in **Figure 2**, shows a tendency of the six different kinds of flours to cluster, even if there is a high degree of overlapping.

Therefore, to improve the separation and to classify quantitatively the analyzed samples, the WPTER algorithm has been used. The best 12 cycles, according to their lowest SF values, have been analyzed in detail; good results were obtained for most of them. Here, two of those best performing classification models are presented, to point out the convergence of the results toward chemically meaningful classification models. The first considered cycle has been obtained by using a biorthogonal 2.4 wavelet, the maximum decomposition level equal to 7, and the percentage of coefficients retained after thresholding equal to 0.5. Fifteen wavelet coefficients have been selected by WPTER for this classification model. **Figure 3a** reports the mean original signal of each class with the selected regions highlighted in dark gray. Two spectral regions have been selected: the first one is a narrow portion centered at about 2850 cm^{-1}, and the second one goes from 2200 to 1400 cm^{-1}. The bands in these regions have been recognized by other authors (*19, 20*) as being typical of lipid and protein components of flours. In particular, the thin bands centered at 2850 cm^{-1} are attributed to symmetric *stretching* vibrational modes of the C−H bond in alkylic CH$_2$ and CH$_3$ groups, and are mainly due to lipids, as is also the peak at 1745 cm^{-1}. The two intense absorption bands that have been selected at about 1650 and 1540 cm^{-1} may be attributed
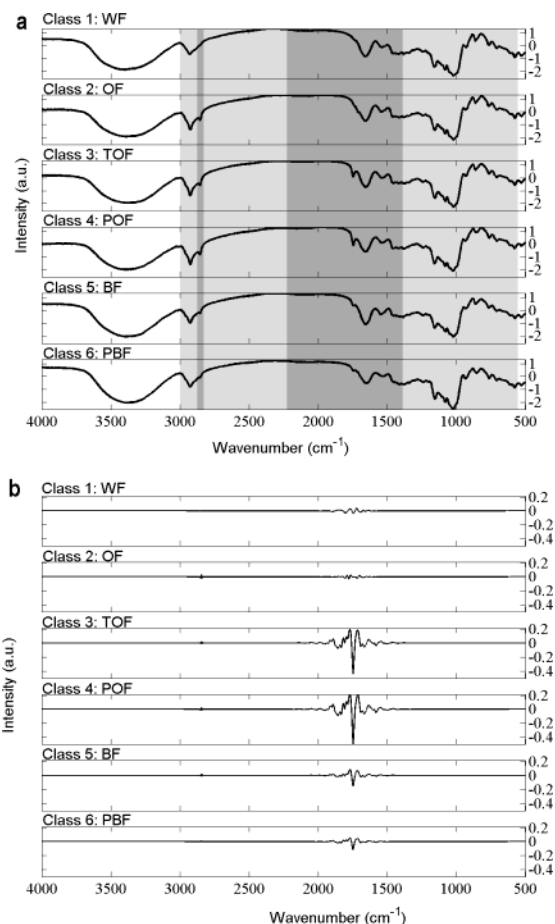

Figure 3. Mean original signals for each class (**a**) the regions corresponding to the selected features by WPTER classification model with bior2.4 are highlighted in light gray, and the region corresponding to the selected features by WPTER classification model with coif3 is highlighted in dark gray. Mean reconstructed signals for each class (**b**) by WPTER classification model with coif3.

to AMIDE I and AMIDE II, respectively. These two absorption bands are associated with combinations of vibrational modes of the amido groups of the amino acids in the proteic structures, and are particularly important, since they reflect modifications of the secondary protein structure (*20*).

The PA bar graphs for the training and for the test sets are reported in **Figure 4a,b**, respectively. All the objects of the training set are correctly assigned to the proper classes, with the only exceptions of signal no. 16, which is assigned both to its own class OF, and partly to class WF, and of signal no. 26, which is only partly assigned to its own class POF. The class assignment of the test set is also satisfactory, with the exception of signal no. 8.

The second classification model that is reported has been obtained by using a coiflet 3 wavelet, the maximum decomposition level equal to 7 and the percentage of coefficients retained after thresholding equal to 0.5%. Ten wavelet coefficients have been selected by WPTER for this classification model. The selected regions, highlighted in light gray in **Figure 3a**, cover the whole spectral range from 3000 to 500 cm^{-1}. However, looking at the corresponding reconstructed signal in **Figure 3b**, it can be noticed that only two portions of this wavenumber range, corresponding to those selected by the previous model, differ significantly from zero. Hence, the two models bring the same chemical information. The bar graph of **Figure 5a** shows
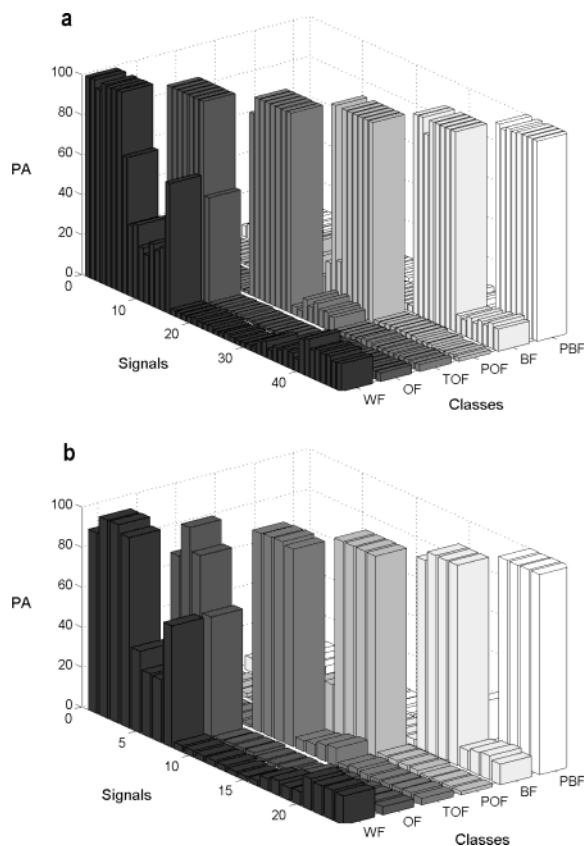
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Figure 4. Percentage of assignation of the training (**a**) and of the test (**b**) set signals, classified according to the WPTER model with a bior2.4 wavelet, maximum decomposition level = 7, percentage of retained coefficients = 0.5.

Figure 5. Percentage of assignation of the training (**a**) and of the test (**b**) set signals, classified according to the WPTER model with a coif3 wavelet, maximum decomposition level = 7, percentage of retained coefficients = 0.5.

that the classification of the training set is analogous to the previous one, while better results have been obtained for the test set; in fact, all the test set signals have been correctly classified (**Figure 5b**).

The effectiveness of the feature selection operated by WPTER was further tested by applying PCA to the wavelet coefficients selected by this classification model. In **Figure 6**, the different pure flours are represented in the space of the first two PCs as circles with different colors. From a comparison of this data distribution with the one of **Figure 2**, it is clear that feature selection in the wavelet domain leads to a better discrimination among the classes, without any overlapping.

Given the good performance of the classification models obtained on the pure flours, we decided to test whether the selected wavelet coefficients may contain useful information, to distinguish mixtures composed by varying percentages of the pure flours, as well. The MIR spectra of the mixtures reported in **Table 1** have been decomposed in the wavelet domain, and the values of the previously selected wavelet coefficients have been obtained. Then, the PC scores have been predicted by the PCA model previously derived for the pure flours. As can be seen in the score plot of **Figure 6**, where the different symbols indicate different percentage compositions, every mixture is placed between the two pure flours from which it is made, and as its composition in a given pure flour increases, its position in the PC space moves toward the location where the pure samples of the same flour are lying. This plot indicates that the proposed method has discriminating capabilities both at qualitative and at semiquantitative levels.
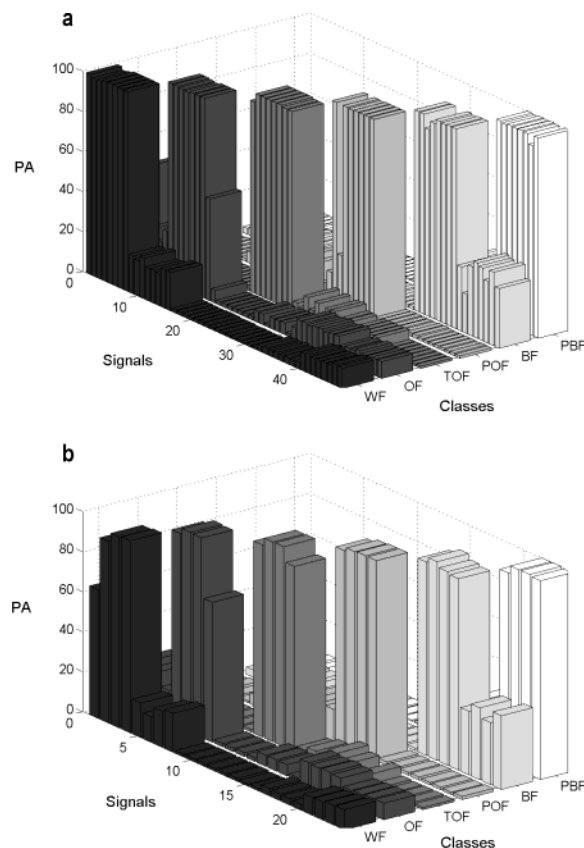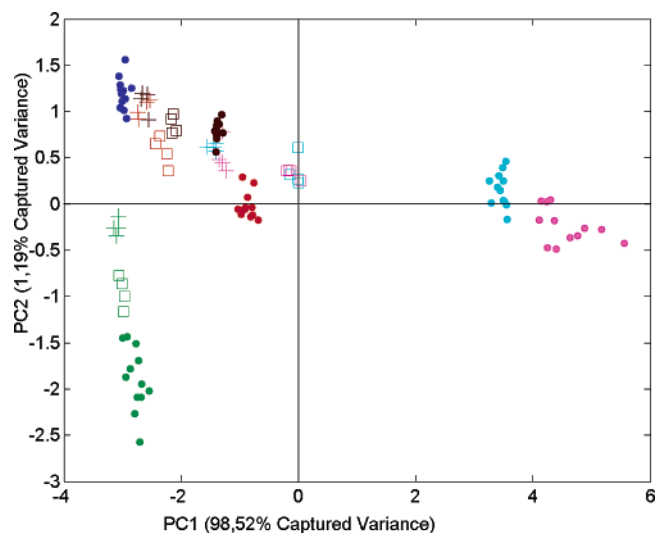

Figure 6. Scores plot of the first two PCs obtained by PCA of the wavelet coefficients selected by the WPTER classification model with a coif3 wavelet, maximum decomposition level = 7, percentage of retained coefficients = 0.5. Filled circles = pure flours; plus signs = mixtures containing 80% WF; squares = mixtures containing 60% WF. The markers colors have been assigned as follows: dark blue for WF, green for OF, cyan for TOF, magenta for POF, red for BF, and brown for PBF.

CONCLUSIONS

The results presented here suggest that the collected MIR spectra contain useful chemical information for discriminating different varieties of cereal flours subjected to different tech-

nological treatments. The WPTER classification results were quite satisfactory both for the training and for the test sets. Moreover, it is worth noticing that in the spectral regions selected by WPTER are located absorption bands, which are chemically meaningful for the studied matrix. In fact, the results of the classification indicate variability in the proteic and lipidic components of flours. This work highlights the usefulness of the proposed approach to better understand and to characterize the flour matrixes. In particular, these results are encouraging in view of studying mixtures of the considered flours, to predict their performances in dough and bread making processes.

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