



# Comparison of artificial neural networks and multiple regression tools applied to near infrared spectroscopy for predicting sensory properties of products from quality labels



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## ABSTRACT

In products from quality labels a sensory analysis is obligatory although this is a slow and expensive process. This study examines the prediction of the sensory parameters of *chorizo* dry-cured sausage by using NIRS technology and the application of chemometric methods such as MPLS (Modified Partial Least Square regression) and ANN (Artificial Neural Networks). The results show that by applying ANN it is possible to predict the 20 sensory parameters analyzed with RSQ values of from 0.61 to 0.92; these values are always higher than those obtained by prediction using MPLS. Moreover, the combination of NIRS and RMS-X residual discrimination allowed the correct classification of 94.4% of the samples according to whether or not they belonged to a certain Quality Label.

## 1. Introduction

In Spain, the dry-cured sausages known as *chorizo* are traditional products of high quality. Some of them, such as the Chorizo de Cantimpalos or the Chorizo Riojano, belong to a Protected Geographical Indication (PGI). This is a concept to assure consumers that the products belonging to them are genuine by providing them with the legal protection of EU Regulation 1151/2012 against misuse or falsification and by guaranteeing the reputation associated with the name. As part of this system for ensuring quality, products allocated to Protected Denominations of Origin (PGI), and other recognized quality labels must undergo sensory analyses to guarantee the authenticity of their attributes. However, at the time of writing no regulations exist on the carrying out of this kind of quality control methods on specific products, with the exception of virgin olive oil which is under EU Regulation 2016/1227. Indeed there are very few examples in the scientific literature of products from quality labels [1,2]. However, considerable efforts are being devoted to the detailed description of how to create a trained panel for the drawing up of sensory profiles [3–5]. These studies reveal that it is necessary to follow multiple stages which are described in widely recognized standards [6]. These stages also include the validation of the panel and all this involves a long period of time.

It is therefore desirable to replace sensory assessment with a more rapid, simpler, and cheaper instrumental analysis such as Near Infrared Spectroscopy (NIRS). This is a technique which has been shown to be very useful for predicting sensory parameters in different matrices such as expanded snacks [7], cheeses of varying composition [8], and fruits [9]. Difficulties have arisen regarding the prediction of the sensory parameters of meat; accuracy is improved with a satisfactory variability of the samples, with a highly trained panel, and with the use of different multivariate techniques to analyze the data [10–12].

Regarding meat products, NIRS technology has been used in the assessment and classification of cooked ham [13] and in the prediction of the sensory quality compliance of dry-cured ham samples [14]. On the other hand, FTIR Imaging (Fourier Transform InfraRed Imaging) has been used to carry out homogeneity studies on Frankfurter sausages [15] and FT-NIR (Fourier Transform Near Infrared Spectroscopy) to predict the basic composition of steamed sausages [16].

Regarding sensory quality, Near Infrared Reflectance (NIR) and Near Infrared Transmittance (NIT) spectroscopy have been indicated as potential methods for the determination of some organoleptic parameters of sausages [17]. However, there are no references on the use of NIR spectroscopy for the prediction of sensory parameters in dry or fermented sausages, although it has been used for the quality control of

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these products. It has been successfully applied in the analysis of majority parameters [18] to determine the pH, color, intramuscular fat, and cutting force [19], to predict the hydroxyproline content [20] and for the rapid detection of irradiation [21]. Indeed some studies have shown that FT-NIR spectroscopy is the most suitable method for the on-line monitoring of the drying process of fermented sausages [22]. In this sense, when benchtop, industrial fiber-optic coupled, and portable FT-NIR were compared for sausage analysis the results showed that benchtop devices give the highest reproducibility and resolution but require the longest measurement times. The FT-NIR linked to a fiber optic probe for on-line determination has the advantage of needing no sample preparation and can be used in adverse environments although it has lower reproducibility and signal intensity. Finally portable devices are cheaper and easier to use but their main disadvantages are their lower reproducibility and higher limits of detection [23].

As has been mentioned, the application of various multivariate methods is essential in NIRS technology. For modeling instrumental-sensory relationships, the classical statistical methods of multivariate analysis such as PLS (Partial Least Squares) or MPLS have been the most widely used. However, these methods are based on the linear dependence of variables, and this situation is not fully applicable to sensory data. In this context, Artificial Neural Networks (ANN) represent an alternative approach for classification and calibration because they are computational techniques that are perfectly suited to the discovering of non-linear trends among variables even when these are unknown; they have been used for predicting the sensory properties of different products such as juices or olive oil [24,25]. However, for the moment we have no record of the use of NIRS in the prediction of the sensory quality of meat products from Quality Label denominations.

The objective of this study is the prediction of the sensory parameters of *chorizo* dry-cured sausages included in the Chorizo de Cantimpalos PGI and the Chorizo Zamorano guarantee label (Quality Labels of food products in Spain) by using NIRS technology and applying chemometric methods. These products are characterized by having a high number of sensory parameters and there are currently no references to the prediction of the complete sensory card of a meat product and specifically of dry-sausages. Two chemometric methods (MPLS and ANN) are compared because although both methods have been previously applied for predicting sensory parameters no studies exist comparing both methods for the purpose. Finally the feasibility of determining whether unknown items belong to these quality labels was investigated, because it is very important for PGIs to clearly authenticate their products and differentiate them from other very similar products and for the moment there is no optimum method for doing this.

## 2. Materials and methods

### 2.1. Samples

In this study we used a total of 72 different samples of *chorizo* from the Chorizo Zamorano guarantee label (36) and the Chorizo de Cantimpalos PGI (22) and 14 samples of *chorizo* not belonging to a Guarantee Label or PGI. The samples were produced according to the ingredients and procedures established by the respective Regulatory Boards. According to the conditions of the Chorizo Zamorano guarantee label therefore, this is a cured raw sausage produced with fresh meat of white-layer fatty pork using the loin, shoulder, ham, belly, lean meat, and streaky bacon with the addition of sweet or spicy paprika belonging to the Pimentón de la Vera Denomination of Origin, salt, garlic, and oregano. The raw materials are chopped up (8 mm to 12 mm opening), mixed with the remainder of the ingredients, left to stand, and stuffed into natural cow or pig gut; the *chorizos* are then kept in a drying room with a relative humidity of between 70 and 85% at a temperature of between 7 and 12 °C for at least four weeks. The product is certified according to European Regulation EN 45011:1998.

The products included in the Chorizo de Cantimpalos PGI are cured sausages made from between 70% and 80% of fresh lean meat of fatty pork to which are added salt and paprika belonging to the Pimentón de la Vera D.O. as basic ingredients with garlic and oregano being optional. It may include sugars, ascorbic acid, citric acid, phosphates, and milk protein. The raw materials are prepared at less than 12 °C with the elimination of fat and tendons; they are chopped up (10 mm to 16 mm opening), mixed with the remainder of the ingredients, and left to stand for 12 to 36 h at a temperature of between 2 and 7 °C. After the stuffing they will be subjected to a curing process of between 21 and 24 days or more; i.e. they will be kept in natural drying rooms at least 40% of the total time.

The products not belonging to quality labels were acquired in shops in the same geographical areas as those of the quality labels; their productive process was similar to that of the latter.

### 2.2. Sensory analysis

The sensory analysis of the samples was carried out by a panel of ten panelists previously selected and trained in the use of Qualitative Descriptive Analysis (QDA) [1]. The panelists were between 20 and 50 years old; 66% were women and 34% were men. All the sessions were held in a laboratory of sensory analysis equipped with individual booths. The advisors were trained in the specific sensory profiling of *chorizo* during 17 sessions lasting 1–1.5 h each. Four sessions were devoted to choosing and defining the sensory parameters and achieving consensus on the methodology of assessment. The panelists subsequently discussed these items during the harmonization sessions. Table 1 shows the final sensory card which included the evaluation of external parameters (assessed in the intact whole product), evaluation of the cutting area, (assessed in a 10-cm section of the sausages cut across their axis), and parameters related to the tasting phase (assessed in 1-cm thick slices taken 3 cm from the end of the sausages), their description and the methodology of assessment.

During the three subsequent sessions (qualification sessions), the panelists assessed the same sample three times each session in order to calculate its reproducibility and repeatability, both by individual panelists and by the panel as a whole [1]. The qualification sessions ended when the maximum uncertainties were lower than 0.5 and 0.8 for repeatability and reproducibility respectively. Subsequently a total of 18 quantification sessions were held in the sensory laboratory, with 4 samples being tasted in each session. The selected sensory parameters were measured using a 9-point scale in which 1 referred to the minimum intensity and 9 to the maximum intensity for each of the attributes.

### 2.3. NIR spectroscopy

The Foss NIR System 5000 monochromator equipment (Foss NIRSystems, Silver Spring, MD) was used. The spectra were registered with a remote reflectance fiber-optic probe of 1.5 m, 210/210 bundle fiber-optic probe (ref no. R6539-A), applied directly to a slice of *chorizo*. The samples are scanned by means of a quartz window of the probe with a surface area of 5 cm × 5 cm. The instrumentation allows the measuring of reflectance in the NIR region in the wavelength range of 1100–2000 with 2 nm of spectral resolution, which implies that 450 data of reflectance were obtained for each sample. Reflectance data were transformed into absorbance by calculating the logarithm of the reciprocal of the reflectance values ( $A = \log 1/R$ ). 3 registers are carried out per sample; each register is the result of the spectrum at 32 different points of said sample and the mean of the 3 registers is used for the study. Fig. 1 shows the spectra of the samples. The software used for spectral collection, data manipulation and chemometric analysis was Win ISI 1.50 (Infrasoft International, State College, PA), installed on a Hewlett-Packard Pentium III computer. The NIRS spectra of the 72 samples were registered, dividing them at random into the calibration

**Table 1**  
Sensory parameters evaluated by the panelists, their definition and Mean, maximum, minimum values and standard deviation of the sensory parameters evaluated in the samples of chorizo dry-sausages.

| Attribute                             | Definition  | Scale   | Minimum | Maximum | Mean | SD   |
|---------------------------------------|---|---|---------|---------|------|------|
| <i>External evaluation</i>            |   |   |         |         |      |      |
| Quality of external odor              | The presence of the typical odor in a balanced way, characterized by hints of paprika, gut and mould without the predominance on any of them. | Not balanced or atypical-Balanced and typical     | 4.00    | 7.56    | 5.92 | 0.85 |
| Intensity of external odor            | The intensity of the overall odor of the sample before cutting  | Slight-Intense                                    | 3.83    | 7.29    | 5.92 | 0.67 |
| Homogeneity of the mould              | The mould is homogeneously distributed in the dry sausage surface   | Heterogeneous-Homogeneous                         | 4.14    | 9.00    | 6.96 | 1.40 |
| External off-odor                     | The intensity of unexpected flavors before cutting  | Slight-Intense                                    | 0.25    | 6.11    | 1.94 | 1.11 |
| <i>Evaluation of the cutting area</i> |   |   |         |         |      |      |
| Easy to remove the casing             | Degree of easiness displayed when removing the casing of the slice  | Difficult-Easy                                    | 0.13    | 8.88    | 6.51 | 1.40 |
| Meat mass binding                     | The level at which the granules of fat and meat are united and the presence of the holes inside   | Low binding big holes- High binding without holes | 4.70    | 7.75    | 6.73 | 0.67 |
| Smearing                              | The level at which the edges of the granules of fat and meat are well defined   | Low-High  | 1.56    | 5.71    | 3.51 | 0.91 |
| Rind dryness                          | The presence of an external dry rind  | Little - A lot                                    | 0.43    | 3.86    | 1.62 | 0.84 |
| Quality of internal odor              | The presence of the balanced and typical odor, slightly acid and characterized by hints of paprika and spices (oregano, garlic).              | Not balanced or atypical-Balanced and typical     | 4.00    | 7.71    | 6.34 | 0.66 |
| Intensity of internal odor            | The intensity of the overall odor of the sample   | Slight-Intense                                    | 4.40    | 7.22    | 6.12 | 0.63 |
| Acid odor                             | The intensity of acid odor  | Slight-Intense                                    | 0.83    | 4.57    | 2.67 | 0.72 |
| Internal off-odor                     | The intensity of unexpected flavors in the slice  | Slight-Intense                                    | 0.13    | 4.56    | 1.03 | 0.81 |
| <i>Evaluation during consumption</i>  |   |   |         |         |      |      |
| Hardness                              | The force necessary to penetrate the meat with the incisors   | Tender - Tough                                    | 3.00    | 7.71    | 4.46 | 1.07 |
| Chewiness                             | The number of times the sample must be chewed before it can be swallowed  | Little - A lot of                                 | 3.17    | 6.89    | 4.77 | 0.90 |
| Juiciness                             | The amount of juice given off by the sample when chewed   | Dry - Juicy                                       | 4.17    | 6.70    | 5.57 | 0.52 |
| Fatness                               | The fatty or lardy sensation in the mouth when chewing the sample   | Little - A lot of                                 | 3.67    | 7.25    | 5.62 | 0.72 |
| Quality of the flavor                 | The presence of the balanced and typical flavour to cured meat, slightly acid and characterized by hints of paprika and spices.               | Not balanced or atypical-Balanced and typical     | 3.86    | 7.50    | 6.11 | 0.70 |
| Intensity of the flavor               | The intensity of the overall flavor of the sample   | Slight-Intense                                    | 5.13    | 7.22    | 6.28 | 0.45 |
| Acid flavor                           | The intensity of acid flavor  | Slight-Intense                                    | 1.14    | 4.10    | 2.36 | 0.77 |
| Off-flavor                            | The intensity of unexpected flavors   | Slight-Intense                                    | 0.22    | 4.86    | 1.22 | 0.95 |

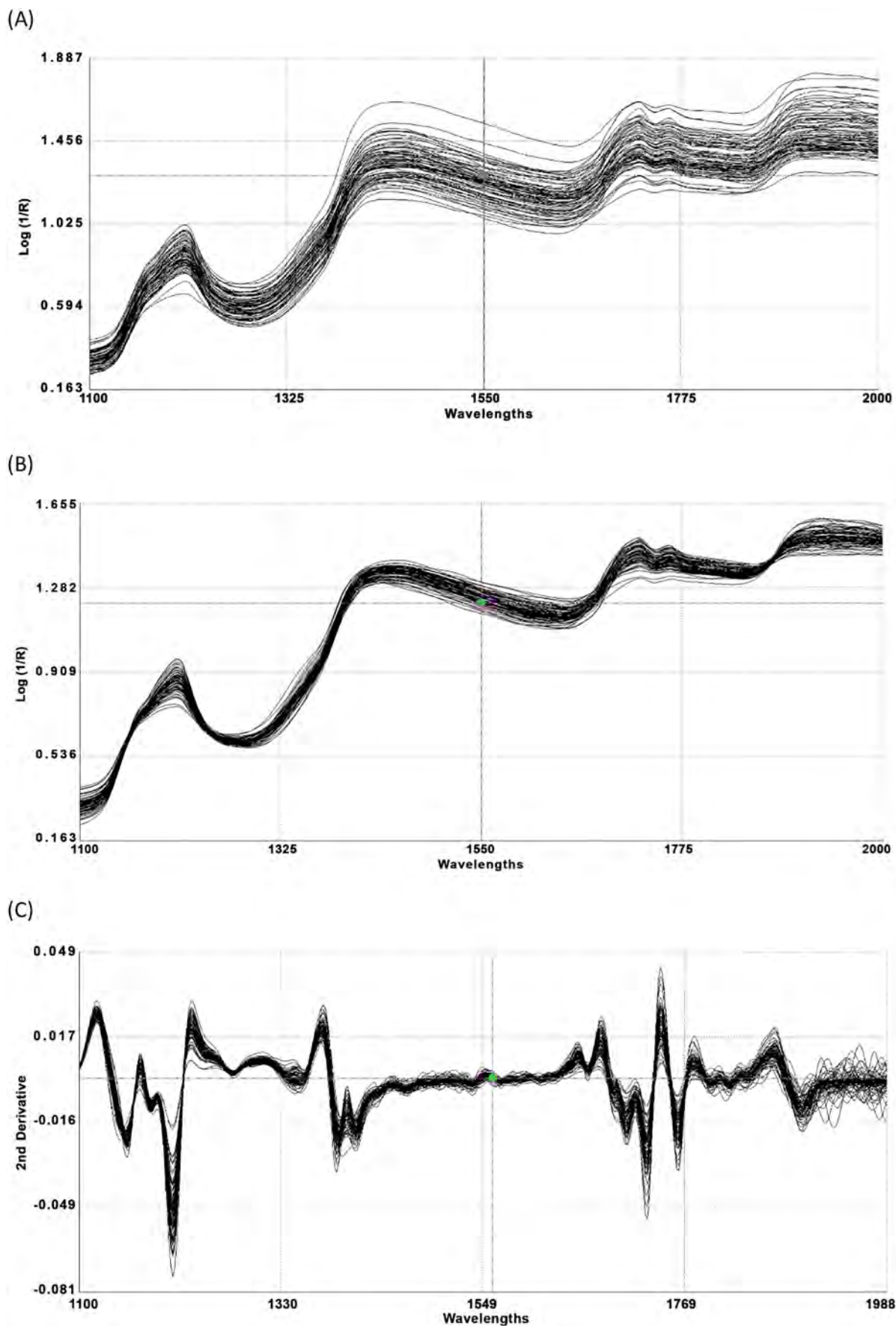


Fig. 1. Plot of the original (a) and pre-processed NIR spectra of 72 samples. (B) Standard MSC 0,0,1,1 (C) None 2,4,4,1; (D) SNV only 2,4,4,1; (E) Standard MSC 2,8,6,1; (F) Detrend only 1,4,4,1.

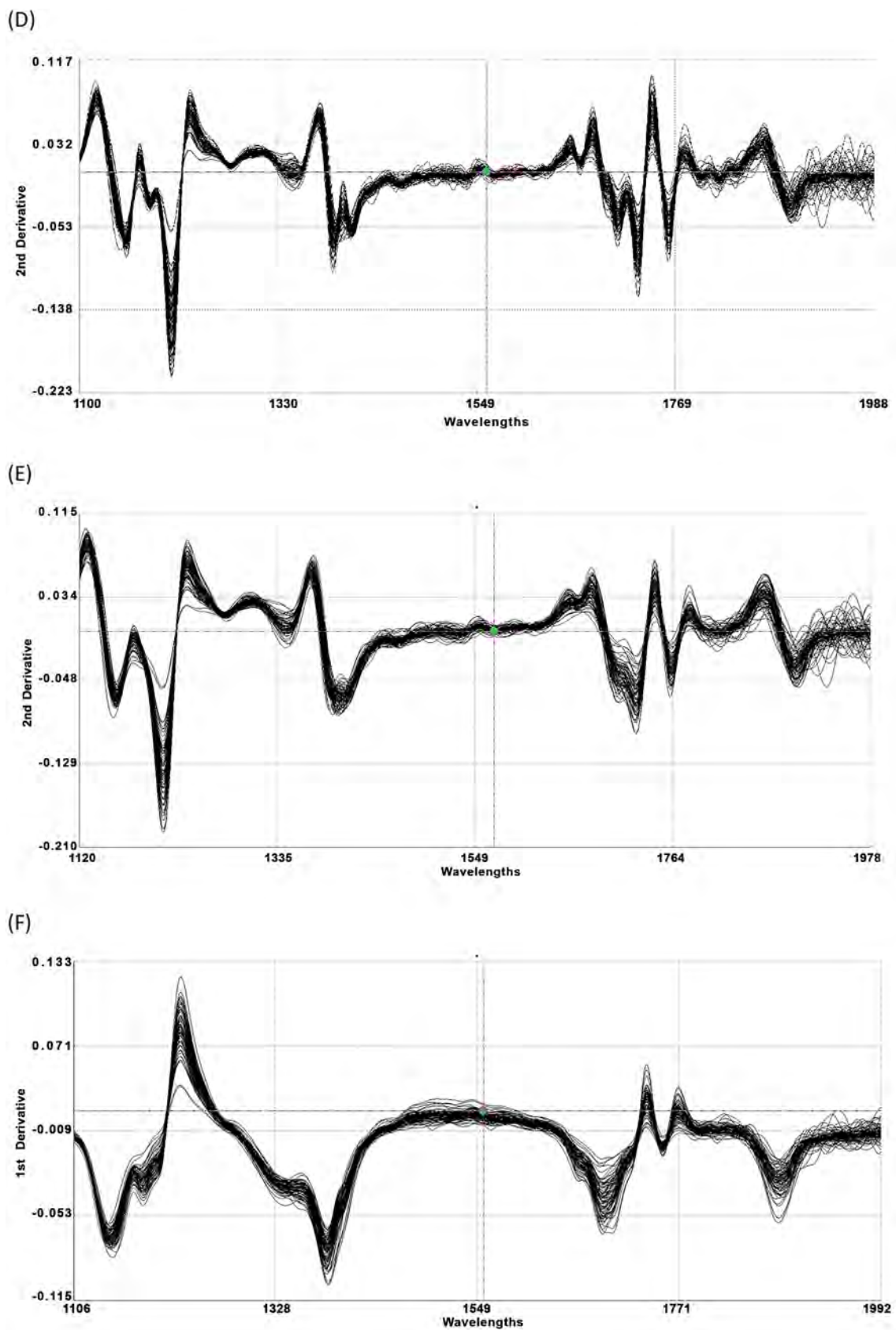


Fig. 1. (continued)

set (58) and the external validation set (14).

#### 2.4. MPLS calibration

The *chorizo* sensory parameters were calibrated by using the MPLS method [8]. The quantification of the different analytical parameters was performed using the modified partial squares (MPLS) regression method. Partial least squares (PLS) regression is similar to principal component regression (PCR) but uses both reference data (chemical, physical, etc.) and spectral information to form the factors useful for suitable purposes [26]. MPLS is often more stable and accurate than the standard PLS algorithm. In MPLS, the NIR residuals obtained after each factor and at each wavelength were calculated and standardized (dividing them by the standard deviations of the residuals at each wavelength) before the next factor was calculated.

For MPLS method, spectra were pre-processed by means of PCA (principal component analysis). Once the number of principal components had been determined, the spectral anomalies were analyzed using the Mahalanobis distance (H statistic) method, establishing a value of  $H = 2.7$  as the upper limit. Samples with an H value of above 2.7 were accordingly considered different from the spectral population and were removed from the set. Another criterion to be considered is the T criterion which is based on chemical parameters (the differences between the sensory panel value and the NIRS-predicted value). Samples with a T value exceeding 2.5 were removed from the set because they were different from the population. Taking into account both H and T criteria, the calibration process was performed with the spectra of the resulting samples and their sensory data.

Scattering effects were removed using multiplicative scatter correction (MSC), standard normal variate (SNV), DeTrend (DT), or SNV-DT. Moreover, the mathematical treatments were tested in the development of the NIRS calibrations by using a nomenclature of 2,4,4,1 in which the first digit is the number of the derivative, the second is the gap over which the derivative is calculated, the third is the number of data points in a running average or smoothing, and the fourth is the second smoothing. The validation was carried out using a cross-validation process. To do so, the set of calibration samples is divided into a series of subsets, in our case 6. Of these, 5 were taken for the calibration set and one for the prediction set. The process is repeated as many times as there are sets, so that all pass through the calibration set and the prediction set. Using this process, we validated the models used and checked their prediction capacities and the statistical parameters obtained are shown in Table 2. The prediction capability of the equation was determined by using the RSQ (R squared) and SECV (Standard error of cross-validation). The values of the different statistical parameters calculated are shown in Table 2.

Finally, the robustness of the method was checked by applying the calibration equations obtained during the work to the NIR spectra of 14

new samples that did not belong to the calibration group, then the predicted values were compared with the reference data. The NIRS methodology and the sensory reference data were compared, using Student's *t*-test for paired values. The p value, the residual mean and the Root Mean Squared Error Values (RMSE) are shown in Table 2.

#### 2.5. Artificial neural networks

The values obtained were processed with ANN feedforward networks of the MLP (Multi Layer Perceptron) type with an input layer with 450 neurons fed with the values obtained in the NIR, another hidden layer with a variable configuration of between 1 and 15 neurons, and an output layer with a single neuron to show the value of each of the sensory parameters. The training algorithm used was the Levenberg-Marquardt Backpropagation algorithm. The Hyperbolic tangent sigmoid and pure linear transfer functions were used in the hidden and output layers respectively. The weight and bias matrix was randomly initialized but by using a known seed value number that allows the reproducibility of data [27]. The expected set of pairs of input-output data was divided at random into a training set (70%), a validation set (15%), and a test set (15%) for all ANN tested. A total of 500 ANN architectures were tested for each sensory parameter in order to find the best one. The prediction capability of the ANN was determined by the higher RSQ and lower RMSE. The root mean square error was calculated as follows

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2}$$

with  $y_i$  being the value observed for each parameter given by the panelists and  $\hat{y}_i$  the predicted value given by the ANN of the *i*-th sample. The software used was the Deep Learning Toolbox of MatLab (MathWorks®) in its R2018 version.

#### 2.6. Discriminating analysis

A discriminating analysis of the geographical origin of samples belonging to the Chorizo de Cantimpalos PGI, the Chorizo Zamorano® Guarantee Label, and samples not belonging to any of these Quality Labels was carried out using the RMS-X residual method (Residual Mean Squares). In this method the square root of the arithmetical mean of the Residual Mean Squares (RMS, or quadratic mean) is calculated to obtain the RMS-X residual values. This measuring is useful when one wishes to detect a spectral variation dissimilar to the spectral variation in the set of data of the products of reference and allows the classification of the samples in several groups. To do so, different mathematical treatments (MSC, SNV, DT or SNV-DT), derivatives, and smoothing procedures were tested in order to find the best discrimination among samples [28]. This analysis was carried out with the Win ISI 1.50

**Table 2**

Descriptors of NIR calibration and results of external validation for the sensory parameters calibrated by MPLS.

| Sensory attribute         | Mathematical treatment | Calibration |      |      |      |      |      |      | External validation |      |               |      |
|---------------------------|------------------------|-------------|------|------|------|------|------|------|---------------------|------|---------------|------|
|                           |                        | N           | SD   | Min  | Max  | Mean | SEC  | SECV | RSQ                 | p    | Residual mean | RMSE |
| External off-odor         | None 2,4,4,1           | 56          | 0.96 | 0.00 | 4.71 | 1.83 | 0.58 | 0.79 | 0.63                | 0.89 | 0.71          | 0.36 |
| Easy to remove the casing | SNV only 2,4,4,1       | 55          | 1.08 | 3.47 | 9.97 | 6.72 | 0.61 | 0.97 | 0.69                | 0.17 | 0.65          | 0.40 |
| Smearing                  | Standard MSC 2,8,6,1   | 57          | 0.93 | 0.75 | 6.31 | 3.53 | 0.45 | 0.66 | 0.76                | 0.78 | 0.69          | 0.40 |
| Rind dryness              | Standard MSC 2,4,4,1   | 55          | 0.79 | 0.00 | 3.89 | 1.53 | 0.53 | 0.63 | 0.55                | 0.25 | 0.65          | 0.20 |
| Acid odor                 | Detrend only 1,4,4,1   | 57          | 0.70 | 0.63 | 4.81 | 2.72 | 0.48 | 0.67 | 0.52                | 0.36 | 0.59          | 0.19 |
| Internal off-odor         | None 2,4,4,1           | 54          | 0.50 | 0.00 | 2.38 | 0.87 | 0.35 | 0.53 | 0.52                | 0.18 | 0.31          | 0.03 |
| Hardness                  | Standard MSC 0,0,1,1   | 57          | 1.08 | 1.29 | 7.76 | 4.52 | 0.56 | 0.74 | 0.73                | 0.46 | 0.53          | 0.21 |
| Chewiness                 | Detrend only 1,4,4,1   | 54          | 0.86 | 2.20 | 7.37 | 4.78 | 0.47 | 0.59 | 0.70                | 0.28 | 0.51          | 0.18 |
| Juiciness                 | SNV only 2,4,4,1       | 56          | 0.50 | 4.10 | 7.10 | 5.60 | 0.25 | 0.50 | 0.75                | 0.59 | 0.35          | 0.05 |
| Acid flavor               | Standard MSC 2,4,4,1   | 56          | 0.74 | 0.11 | 4.53 | 2.32 | 0.40 | 0.61 | 0.71                | 0.78 | 0.57          | 0.20 |

N: number of samples, SD: Standard Deviation, SEC: Standard Error of Calibration, SECV: Standard Error of cross-validation, RSQ: Multiple correlation coefficient, MSC: Multiple Scatter Correction, SNV: Standard Normal Variate, p: significance level, RMSE: Root Mean Standard Error.

(Infrasoft International, State College, PA).

## 2.7. Model optimisation

The MPLS models are optimized according to the following process: firstly the models with the fewest errors of calibration (SEC) are chosen and subsequently those with the smallest difference between the errors of calibration and prediction (SEP) and highest RSQ values.

The ANN models are optimized by choosing the architecture with the highest RSQ value. If several ANNs show the same RSQ value the network with the lowest number of neurons in the hidden layer will be chosen, as the lower the number of neurons the greater the tendency to lose the generalization capacity by overfitting.

In the case of discrimination using the RMS-X residual method, as in the case of calibrating by MPLS, that combination of mathematical treatment (MSC, SNV, DT or SNV-DT) and the number of derivatives are chosen and the gap over the derivative is calculated together with the number of data points in a running average or smoothing and the second smoothing (for example SNV 2,4,4,1) which gives the highest percentage of correctly classified samples.

## 3. Results and discussion

The NIR spectra of the samples are presented in Fig. 1a with four regions of higher absorbance in the ranges of 1150–1200 nm, 1400–1450 nm, and 1700–1800 nm, and at 1900 nm. These regions were improved by mathematical treatments (Fig. 1b–f) as has been reported in fermented sausages [21].

The mean, minimum, and maximum results together with the standard deviation of the 20 sensory parameters analyzed are shown in Table 1. The parameters analysed were divided into three groups in accordance with their assessment by the samplers. The parameters of external assessment are applied to intact items; they are related to the impression of the consumer on purchase and defined in the sensory card of Quality Labels. According to these Labels the optimum value for the quality of the external odor and its intensity is approximately 5 points which justifies the mean values observed and the low SD. However, in the case of external off-odor the lower the punctuation the higher the quality of the samples. Despite this, some samples showed abnormal odors that were described by assessors as moldy, musty, stable, medicament, or boar taint as previously described for dry fermented sausages [29].

As for the parameters evaluated for the cutting area, some of the chosen parameters were related to the general appearance such as meat mass binding. This parameter has been previously described as a fat/lean connection and selected as one of the main attributes for fermented sausage description [29]. Other relevant parameters were related to the existence of defects such as the ease of removal of the casing, smearing, and rind dryness. The optimum value for the former according to Quality Labels is about 5 points (stuck on but not difficult to remove) although other studies have reported lower values [30]. The presence of a crust or rind dryness is typical of these products [31] and a suitably low value can be observed in the samples analyzed (mean value 1.62). Smearing is not desirable because there must be a well-defined separation between fat and lean meat [29]. The results show that there was a significant variability of this parameter ranging from 1.5 to 5.7. Some odor parameters were also assessed on the surface of the slice and the optimum value for quality and odor intensity was approximately 5 (with mean values of 6.34 and 6.12 respectively). It is noteworthy that *chorizo* Zamorano is characterized by a slight albeit desirable acid odor due to the presence of lactic acid. This acid produces a sour taste without other aromatic touches [32]. This is the reason why the assessors selected an acid odor instead of a lactic odor as previously reported [29]. The values observed were slightly higher than those reported for other types of Spanish *chorizo* [33]. As far as off-odor is concerned, those most frequently found by the assessors were those

previously mentioned together with a rancid odor. This parameter has also been previously described for fermented and dry sausages and shows values ranging from 1 to 5 [30,34].

Finally, assessment during consumption included texture and flavor parameters. Texture parameters such as hardness, chewiness, juiciness, and fatness are usually selected to describe dry sausages [29,31,35]. The mean values of these parameters depended on the product assessed and ranged between 2 and 3 and 7 [35–37]. The results of this study were therefore within the range of variability reported for these products.

At this stage the chosen flavor parameters were similar to those assessed for odor description, showing similar mean values and SD. The use of similar words to describe odor and flavor (aroma) attributes was previously reported [29]. As for the acid odor, although the values of an acid flavor were higher than those previously reported for Spanish *chorizo* the intensity of the flavor was within the range reported by other studies [36]. As for external and internal off-odor the observed values were low and the most abnormal flavors described were rancid.

Taking into account the ranges of variability of the results, it allows a sufficiently wide diversity so as to be able to guarantee that the calibration with NIR spectroscopy is carried out correctly.

### 3.1. Calibration of sensory parameters using the MPLS method

By using the matrix of sensory data and the NIR spectra of the samples, the best equations were optimized by modified partial least square (MPLS) regression. For this purpose, of the total of 72 samples 58 made up the calibration set with which the calibration equations were calculated and the 14 remaining samples constituted the external validation set. Of the 20 parameters assessed in the sampling session only 11 presented values of RSQ > 0.5; these are shown in Table 2 together with the statistical parameters of calibration. After the PCA analysis the number of major components necessary for explaining over 98% of the variability was as follows: 7 for an acid flavor; 8 for the parameters of gut separation, smearing, rind dryness, internal off-odors, acid flavor, and off-flavors; 9 for external off-flavors and juiciness; and 10 for hardness and chewiness. The number of samples eliminated by criterion  $H > 2.7$ , which indicates how different the spectrum of the sample is from the mean spectrum of the population, were 4 samples for chewiness, 2 samples for juiciness, 1 sample for the parameters of smearing, rind dryness, the ease of removal of the casing, an acid flavor, hardness, an internal off-odor, and an acid flavor. In the case of the remainder of the parameters calibrated no sample was eliminated according to this criterion. As for the T criterion 3 samples were eliminated owing to internal off-odor, 2 samples owing to external off-odor, the ease of removal of the casing, and rind dryness while only 1 sample was eliminated owing to smearing, an acid odor, and an acid flavor. The samples eliminated were different depending on the parameter. Table 2 therefore includes the number of samples (N) which were finally used for calibration, the interval in which the calibration equations may be used (Min-Max), and the SECV and RSQ calibration parameters.

The results show that the margins of applicability of the equations obtained by the NIR method in *chorizo* for the parameters of smearing, hardness, chewiness, juiciness, and acid flavor are greater than those included in the reference method in this study. For the parameters of rind dryness, acid odor, internal off-odor, and off-flavor the ranges of application of both methods are similar. Only the parameters of smearing, an acid flavor, and the texture parameters show RSQ values exceeding 0.7.

The validity of the calibration method is checked by means of internal validation or cross-validation, assessing the RSQ parameters (multiple correlation coefficient), SEP (standard error of prediction), and SEPC (standard error of prediction corrected by bias). SEP and SEPC values must be as close as possible and the RSQ value > 0.5. As this condition is not met for the internal off-odor the equation obtained cannot be used to predict this parameter and is not shown in Fig. 2. The

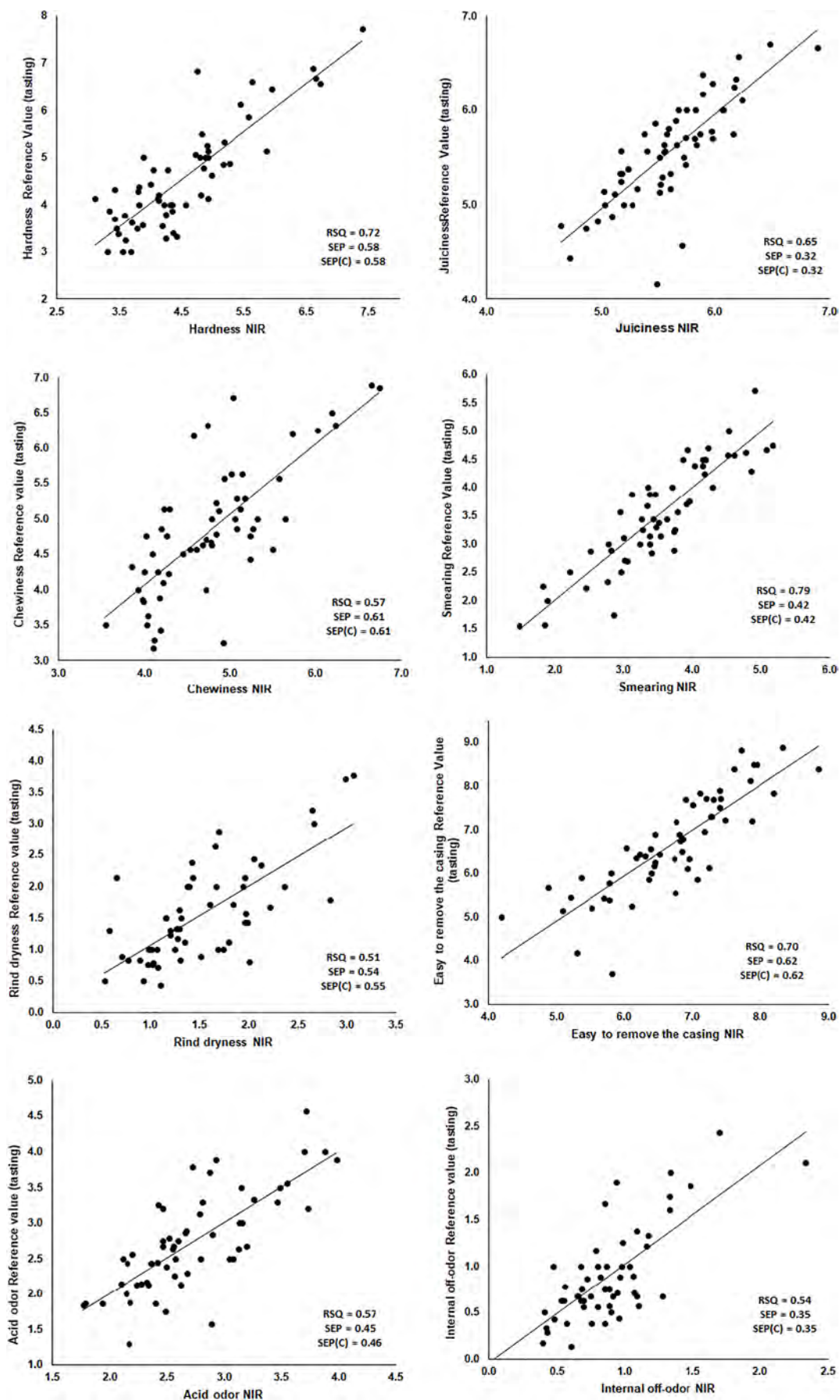


Fig. 2. Comparison of the reference values with the values predicted by MPLS calibration and statistical parameters of MPLS internal validation.

internal validation data show that the parameters of easy to remove the casing, smearing, and hardness present RSQ values higher than 0.7. It is noteworthy that although internal off-odor presented low values it was possible to calibrate this parameter. This was because although the data showed low variability and low values it is well known that the compounds responsible for odor are aldehydes, ketones and alcohols with a very high response in NIR spectroscopy. The off-odors more frequently described by assessors were thus as follows: moldy related to the presence of 1-octen-3-ol [38], stable caused by 4-methyl-phenol [39], and boar taint produced by skatole.

As for the RSQ values found in this study, they are similar to or higher than those indicated by other authors. Other authors reported a RSQ (calibration) of 0.58 and 0.50 for chewiness and juiciness of beef steaks respectively [40]; while others found an RSQ of  $> 0.5$  only for tenderness (RSQ cal = 0.56) [10] similar to that obtained in other works for this parameter (RSQ cal = 0.55) [41]. Other reports showed an RSQ of 0.83 for lamb flavor [42] and other found an RSQ of 0.98 for beef tenderness [11]; however, the remainder of the sensory parameters had an RSQ of less than 0.55. More recently other regression methods such as MLR (Multiple Linear Regression) have given RSQ values similar to those found for MPLS in the assessment of loin pork ranging from 0.57 for hardness to 0.84 for juiciness [43]. As far as meat products are concerned, it has been possible to predict the pastiness (RSQ cal = 0.94) and the color (RSQ cal = 0.66) of dry-cured ham [12]. The number of parameters which it has been possible to calibrate (RSQ  $> 0.5$ ) in this study by MPLS is much higher than those found in all the studies mentioned above.

During the external validation the NIR model is checked against 14 samples of *chorizo* which have not been part of the calibration set. In order to do so the results obtained by applying the prediction equations to the NIRS spectra of these samples are compared with the results given by the panel using the Student's *t*-test for paired values. The results (Table 2) show that there were no significant differences ( $p > 0.05$ ) between both sets for any of the parameters, which indicates that both methodologies give equivalent results. The Root Mean Standard Error (RMSE) values were between 0.05 for the acid flavor and 0.40 for gut separation. From these results it can be concluded that the prediction equations were satisfactory.

### 3.2. Calibration of sensory parameters using Artificial neural networks

At this stage we predicted the sensory parameters by using the Artificial Neural Network methodology. In order to use neural networks, in the first place it is necessary to choose the appropriate training algorithm and network architecture so as to avoid wasting time and effort in the process [44]. Previous research has shown that for the prediction of sensory parameters the most suitable is the Levenberg-Marquardt Backpropagation algorithm, using the Hyperbolic Tangent Sigmoid transfer function for the hidden layer and the Linear Function for the output layer as has been indicated [45]. With this algorithm the percentage of networks (of the total of the trained networks) giving an RSQ value of over 0.7 is higher than that obtained with other training algorithms.

To optimize the network the data were divided into the training set with 50 samples, the validation set with 11 samples and the test set with 11 samples. For each sensory parameter the training was carried out by using the training set to obtain the predicting neural network, the accuracy of which is given by RSQ; afterwards the validation set is used to avoid overfitting of the network and the reduction of its generation capacity. Finally, the performance of the ANN is validated by the test set, i.e. a set of new data not used previously. After running the test set, a new RSQ value and the RMSE is obtained which allow the selection of the best trained network.

This process was repeated using a different number of neurons in the hidden layer (from 1 to 15) in order to ascertain the best architecture. Moreover, for each architecture up to 500 training sessions

**Table 3**

Number of neurons in the hidden layer, RSQ and Root Mean Squared Error (RMSE) of the best ANN architecture for each sensory attribute.

| Attribute                             | Neurons | RSQ  | RMSE |
|---------------------------------------|---------|------|------|
| <b>External evaluation</b>            |         |      |      |
| Quality of external odor              | 15      | 0.67 | 0.50 |
| Intensity of external odor            | 4       | 0.81 | 0.30 |
| Homogeneity of the mould              | 10      | 0.70 | 0.78 |
| External off-odor                     | 1       | 0.77 | 0.61 |
| <b>Evaluation of the cutting area</b> |         |      |      |
| Easy to remove the casing             | 2       | 0.75 | 0.73 |
| Meat mass binding                     | 9       | 0.71 | 0.38 |
| Rind dryness                          | 15      | 0.79 | 0.39 |
| Smearing                              | 15      | 0.84 | 0.37 |
| Quality of internal odor              | 5       | 0.74 | 0.34 |
| Intensity of internal odor            | 7       | 0.61 | 0.40 |
| Acid odor                             | 9       | 0.80 | 0.32 |
| Internal off-odor                     | 5       | 0.87 | 0.29 |
| <b>Evaluation during consumption</b>  |         |      |      |
| Hardness                              | 7       | 0.92 | 0.31 |
| Chewiness                             | 1       | 0.87 | 0.32 |
| Juiciness                             | 3       | 0.81 | 0.25 |
| Fatness                               | 2       | 0.68 | 0.41 |
| Quality of the flavor                 | 1       | 0.73 | 0.38 |
| Intensity of the flavor               | 9       | 0.87 | 0.18 |
| Acid flavor                           | 1       | 0.82 | 0.33 |
| Off-flavor                            | 1       | 0.82 | 0.41 |

were carried out with known seed values which allowed different values to be randomly assigned to the initial weights. It has previously been found that the higher the number of trained networks, the better the performance of the selected ANN (the better the ANN performs the better it predicts). The best ANN architecture for each sensory parameter, which is that given by the higher RSQ value, is shown in Table 3.

The results reveal that the RSQ values ranged from 0.61 for the intensity of the internal odor to 0.92 for hardness. As for the parameters of external assessment, a satisfactory correlation can be observed between the values of reference and those predicted by the network with RSQ values close to or higher than 0.70. It should be stressed that the NIR spectrum was taken from the interior of the slice and that these parameters correspond to perceptions of the exterior of the same. In the parameters relating to perception of the cutting, that with the strongest correlation between the values observed and those predicted was the internal off-odor with an RSQ value of 0.87. On the other hand, the lowest RSQ was shown by the intensity of internal odor, which was moreover the lowest of all the parameters assessed. Finally, the parameters determined during tasting were in general the highest correlation coefficients of those determined in this study, with the exception of fatness. Hardness was therefore the parameter with the highest value (RSQ = 0.92), while chewiness and flavor intensity reached values of 0.87.

The use of neural networks to predict sensory parameters is less generalized. It has been used for the assessment of tenderness [46–48], and color [49–51] when using other techniques such as computer vision or image texture analysis as input data.

### 3.3. Comparison of MPLS and ANN results

If the results obtained by means of MPLS and ANN are compared, it can be observed that by using neural networks it was possible to predict the 20 sensory parameters by means of an RSQ  $> 0.6$  criterion; moreover, the parameters with an RSQ of  $> 0.8$  were 10, which is the number of parameters which it was possible to predict by using MPLS.

This result coincides with that of previous studies which indicate that neural networks provide better adjustments than multiple regression models, for example to predict performance both during lactation [52] and in the production of seeds [53] or in the prediction of quality

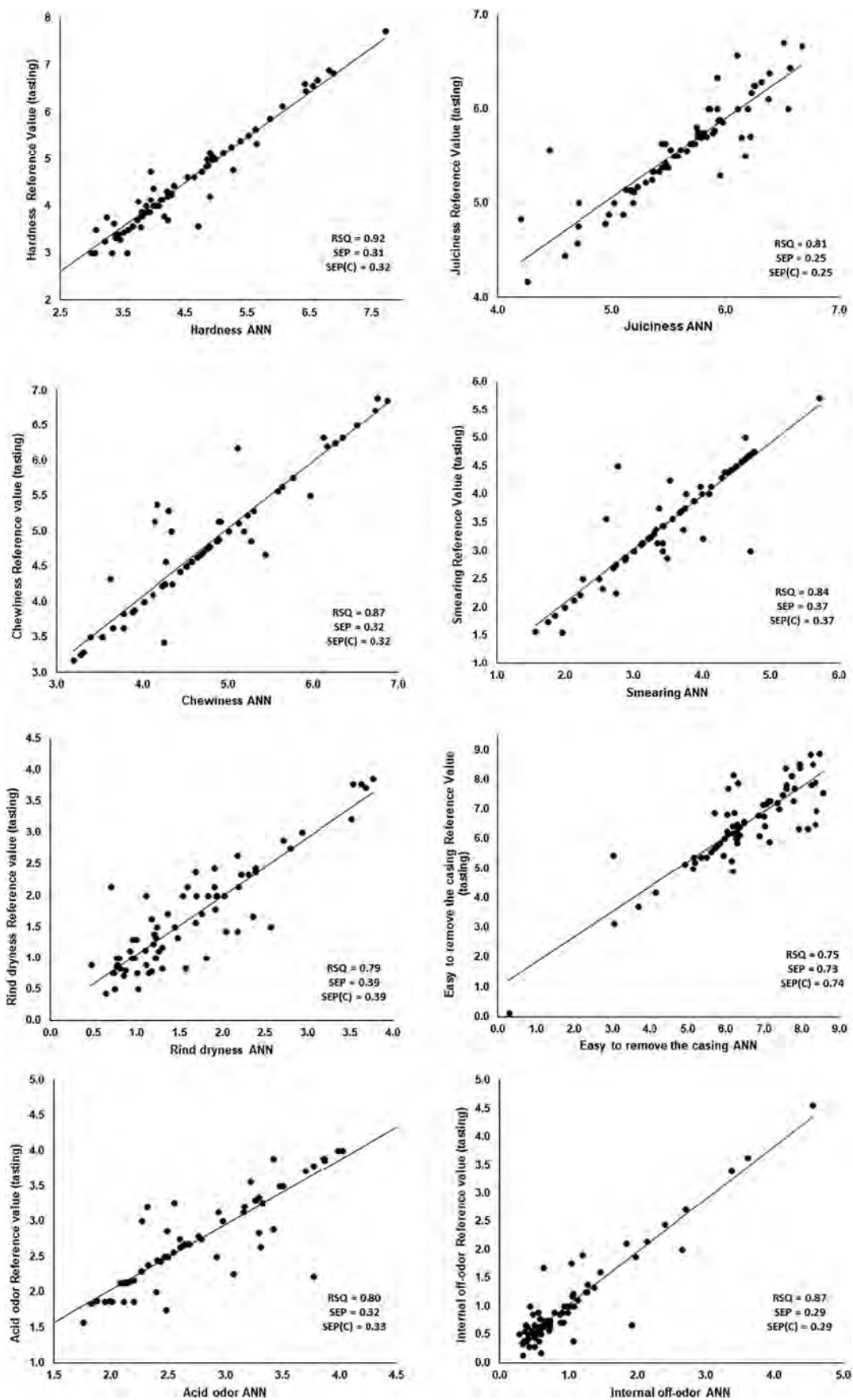


Fig. 3. Comparison of the reference values with the values predicted by ANN calibration.

**Table 4**  
Mean values (+SD) of the sensory parameters evaluated in chorizo dry-sausages according to whether they belong to a certain Quality Label.

| Attribute                             | PGI Chorizo Cantimpalos |        | QL Chorizo Zamorano |        | Others             |        | p     | SEM  |
|---------------------------------------|-------------------------|--------|---------------------|--------|--------------------|--------|-------|------|
| <i>External evaluation</i>            |                         |        |                     |        |                    |        |       |      |
| Quality of external odor              | 6.33 <sup>b</sup>       | ± 0.61 | 5.82 <sup>ab</sup>  | ± 0.93 | 5.53 <sup>a</sup>  | ± 0.72 | 0.012 | 0.10 |
| Intensity of external odor            | 6.07                    | ± 0.59 | 5.89                | ± 0.72 | 5.74               | ± 0.62 | 0.328 | 0.08 |
| Homogeneity of the mould              | 7.80 <sup>b</sup>       | ± 1.31 | 6.58 <sup>a</sup>   | ± 1.28 | 6.62 <sup>a</sup>  | ± 1.33 | 0.002 | 0.16 |
| External off-odor                     | 1.34 <sup>a</sup>       | ± 0.48 | 2.26 <sup>b</sup>   | ± 1.31 | 2.05 <sup>ab</sup> | ± 0.89 | 0.007 | 0.13 |
| <i>Evaluation of the cutting area</i> |                         |        |                     |        |                    |        |       |      |
| Easy to remove the casing             | 6.76                    | ± 2.10 | 6.38                | ± 0.90 | 6.45               | ± 1.15 | 0.589 | 0.17 |
| Meat mass binding                     | 6.96                    | ± 0.53 | 6.61                | ± 0.78 | 6.70               | ± 0.47 | 0.144 | 0.08 |
| Rind dryness                          | 4.07 <sup>b</sup>       | ± 0.59 | 3.24 <sup>a</sup>   | ± 0.99 | 3.31 <sup>a</sup>  | ± 0.73 | 0.001 | 0.11 |
| Smearing                              | 1.45                    | ± 0.92 | 1.57                | ± 0.72 | 2.04               | ± 0.93 | 0.105 | 0.10 |
| Quality of internal odor              | 6.50                    | ± 0.53 | 6.19                | ± 0.74 | 6.44               | ± 0.62 | 0.193 | 0.08 |
| Intensity of internal odor            | 6.17                    | ± 0.54 | 6.04                | ± 0.74 | 6.25               | ± 0.44 | 0.524 | 0.07 |
| Acid odor                             | 2.32 <sup>a</sup>       | ± 0.62 | 2.86 <sup>b</sup>   | ± 0.73 | 2.76 <sup>ab</sup> | ± 0.71 | 0.018 | 0.09 |
| Internal off-odor                     | 0.71 <sup>a</sup>       | ± 0.53 | 1.25 <sup>b</sup>   | ± 0.89 | 0.95 <sup>ab</sup> | ± 0.82 | 0.042 | 0.10 |
| <i>Evaluation during consumption</i>  |                         |        |                     |        |                    |        |       |      |
| Hardness                              | 4.14                    | ± 1.00 | 4.68                | ± 1.08 | 4.39               | ± 1.08 | 0.181 | 0.13 |
| Chewiness                             | 4.37 <sup>a</sup>       | ± 0.81 | 4.99 <sup>b</sup>   | ± 0.88 | 4.85 <sup>b</sup>  | ± 0.93 | 0.034 | 0.11 |
| Juiciness                             | 5.60                    | ± 0.41 | 5.48                | ± 0.61 | 5.74               | ± 0.38 | 0.276 | 0.06 |
| Fatness                               | 5.82                    | ± 0.47 | 5.52                | ± 0.77 | 5.59               | ± 0.91 | 0.305 | 0.09 |
| Quality of the flavor                 | 6.32                    | ± 0.48 | 6.04                | ± 0.77 | 5.95               | ± 0.80 | 0.225 | 0.08 |
| Intensity of the flavor               | 6.12                    | ± 0.40 | 6.31                | ± 0.45 | 6.43               | ± 0.46 | 0.100 | 0.05 |
| Acid flavor                           | 1.74 <sup>a</sup>       | ± 0.42 | 2.72 <sup>b</sup>   | ± 0.73 | 2.42 <sup>b</sup>  | ± 0.74 | 0.000 | 0.09 |
| Off-flavor                            | 0.91                    | ± 0.52 | 1.43                | ± 1.13 | 1.19               | ± 0.84 | 0.123 | 0.11 |

PGI: Protected Geographical Indication, QL: Quality Label, SEM: Standard Error Mean.

parameters of fruits [54]. However, other studies have found that ANN only showed a slightly better performance than the partial least squares regression models (PLS models) for the prediction of cheese texture [55] or even similar results for the prediction of meta composition parameters [56]. This result differs from that obtained in this study in which the ANN performance was significantly better than the MPLS performance. This fact can be clearly observed in Fig. 3 which shows the comparison of the reference values with the values predicted by ANN calibration for those parameters which were predicted by MPLS. The SEP and SEP (C) values were also shown in Fig. 3. The results showed higher RSQ and lower SEP and SEP(C) values for ANN calibration than for MPLS in the ten parameters predicted by both methods, which demonstrates the better performance of ANNs for the prediction of sensory parameters. This is due to the fact that the relationship between physicochemical and sensory responses is probably not linear, and that ANNs are perfectly suited to this purpose because they use non-linear functions in their architecture.

However, examination of the results also reveals that in general the RMSE values (for all the samples) were higher when neural networks were used than when the RMSE values were calculated for the test set in MPLS. However, other studies reported lower values of RMSE for ANN than for linear regression models [53].

### 3.4. Discrimination of samples according to their origin

A analysis of the NIR spectra was then carried out with the aim of distinguishing the samples according to their origin, i.e. whether the sample analyzed belongs to the Chorizo de Cantimpalos GPI, the Chorizo Zamorano Guarantee Label, or the third group known as other. In order to do so the data from the NIR spectrum were pre-treated by the correction of the SNV 2,4,4,1 diffusion and then the model for distinguishing RMS-X residuals was applied. The results obtained show that 20 of the 22 *chorizo* samples of the Cantimpalos PGI were classified correctly, which means a 90.9% success rate. 100% of the samples of the Chorizo Zamorano Quality Label and 12 of the 14 samples of *chorizo* made in Zamora but not belonging to a quality label were classified correctly, and the other two were classified as chorizo belonging to the quality label, which means a success rate of 85.7%. As a whole the success rate of the procedure was 94.4%, which indicates that the

combination of the NIRS methodology with this multivariate analysis can be a highly efficient tool for distinguishing samples according to origin. This result confirms the findings of previous studies which have shown the usefulness of NIRS for distinguishing products as to whether they belong to a PGI or not [57–59].

The analysis of the results given by the panelists according to the origin of the samples (Table 4) made it possible to establish that there were significant differences in 8 of the 20 parameters studied. *Chorizos* from the Cantimpalos PGI were characterized by higher quality as to external odor, greater homogeneity of mould on the surface, greater smearing, less odor and acid flavor, and lower hardness and chewiness. For their part, *chorizos* from the Zamorano Guarantee Label were characterized by having lower values of homogeneity of mould and smearing, while they had the highest values of both external and internal off-odors and acid odors together with the highest values of hardness and chewiness. *Chorizos* not belonging to any quality label were characterized by having the lowest quality values of external odor and similar values of homogeneity of mould, smearing, and acid flavor to the Chorizo Zamorano.

## 4. Conclusion

From the results obtained in this study we conclude that the spectral information of NIRS together with the application of chemometric tool methods allow the predicting of 10 out of 20 sensory parameters of *chorizo* using MPLS and all the sensory parameters assessed using ANNs. In addition, ANNs showed higher RSQ for all the parameters studied. In addition, the use of NIR spectrometry in combination with the RMSX-residuals method allowed the distinguishing of *chorizo* samples according to their origin with a success rate of 94.4% for the samples as a whole. These results reveal the usefulness of NIR spectrometry combined with the appropriate chemometric tool for distinguishing and predicting the sensory profile of samples belonging to Quality Labels.

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## CRedit authorship contribution statement

**Miriam Hernández-Jiménez:** Validation, Formal analysis. **Pedro Hernández-Ramos:** Formal analysis. **Iván Martínez-Martín:** Investigation, Formal analysis. **Ana M. Vivar-Quintana:** Visualization, Writing - original draft. **Inmaculada González-Martín:** Methodology, Validation. **Isabel Revilla:** Conceptualization, Writing - review & editing.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.microc.2020.105459>.

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