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Determination of fat content in chicken hamburgers using NIR spectroscopy and the Successive Projections Algorithm for interval selection in PLS regression (iSPA-PLS)

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ABSTRACT

Determining fat content in hamburgers is very important to minimize or control the negative effects of fat on human health, effects such as cardiovascular diseases and obesity, which are caused by the high consumption of saturated fatty acids and cholesterol. This study proposed an alternative analytical method based on Near Infrared Spectroscopy (NIR) and Successive Projections Algorithm for interval selection in Partial Least Squares regression (iSPA-PLS) for fat content determination in commercial chicken hamburgers. For this, 70 hamburger samples with a fat content ranging from 14.27 to 32.12 mg kg^{-1} were prepared based on the upper limit recommended by the Argentinean Food Codex, which is 20% (w w^{-1}). NIR spectra were then recorded and then preprocessed by applying different approaches: base line correction, SNV, MSC, and Savitzky-Golay smoothing. For comparison, full-spectrum PLS and the Interval PLS are also used. The best performance for the prediction set was obtained for the first derivative Savitzky-Golay smoothing with a second-order polynomial and window size of 19 points, achieving a coefficient of correlation of 0.94, RMSEP of 1.59 mg kg^{-1}, REP of 7.69% and RPD of 3.02. The proposed methodology represents an excellent alternative to the conventional Soxhlet extraction method, since waste generation is avoided, yet without the use of either chemical reagents or solvents, which follows the primary principles of Green Chemistry. The new method was successfully applied to chicken hamburger analysis, and the results agreed with those with reference values at a 95% confidence level, making it very attractive for routine analysis.

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1. Introduction

Foods of animal origin are excellent sources of high quality protein, whose energy value depends mainly on this group of nutrients and also on the amount and quality of fat content. Furthermore, taste and texture of food products depend on fat composition [15]. Among foods of animal origin, hamburgers deserve special attention since they are included in the eating habits of children and teenagers and they require simple preparation. Their consumption is quite large. For example, some fast-food chains such as McDonald's report to have sold about twelve hamburgers per capita around the world. Furthermore, on average, a person living in the United States consumes three burgers per week.

From the nutritional point of view, hamburgers provide protein, fat, vitamins and minerals. Fat content in hamburgers depends mainly on the type of animal used for its manufacture. In the case of prepared hamburgers with chicken meat, they usually have fewer calories than beef hamburger [12,16]. The high consumption of saturated fatty acids and cholesterol is mainly responsible for cardiovascular diseases and obesity [23,26]. The Food and Drug Administration (FDA) requires the declaration of the amount of fatty acids present in foods on their nutrition label [25]. The Argentinean Food Codex (Article 330) established that the amount of fat in hamburgers should not exceed 20% (w w^{-1}) [2]. The fat content determination in hamburgers is required to ensure the quality of the product. In literature, the official Soxhlet extraction method recommended by the AOAC [18] is widely used for determining

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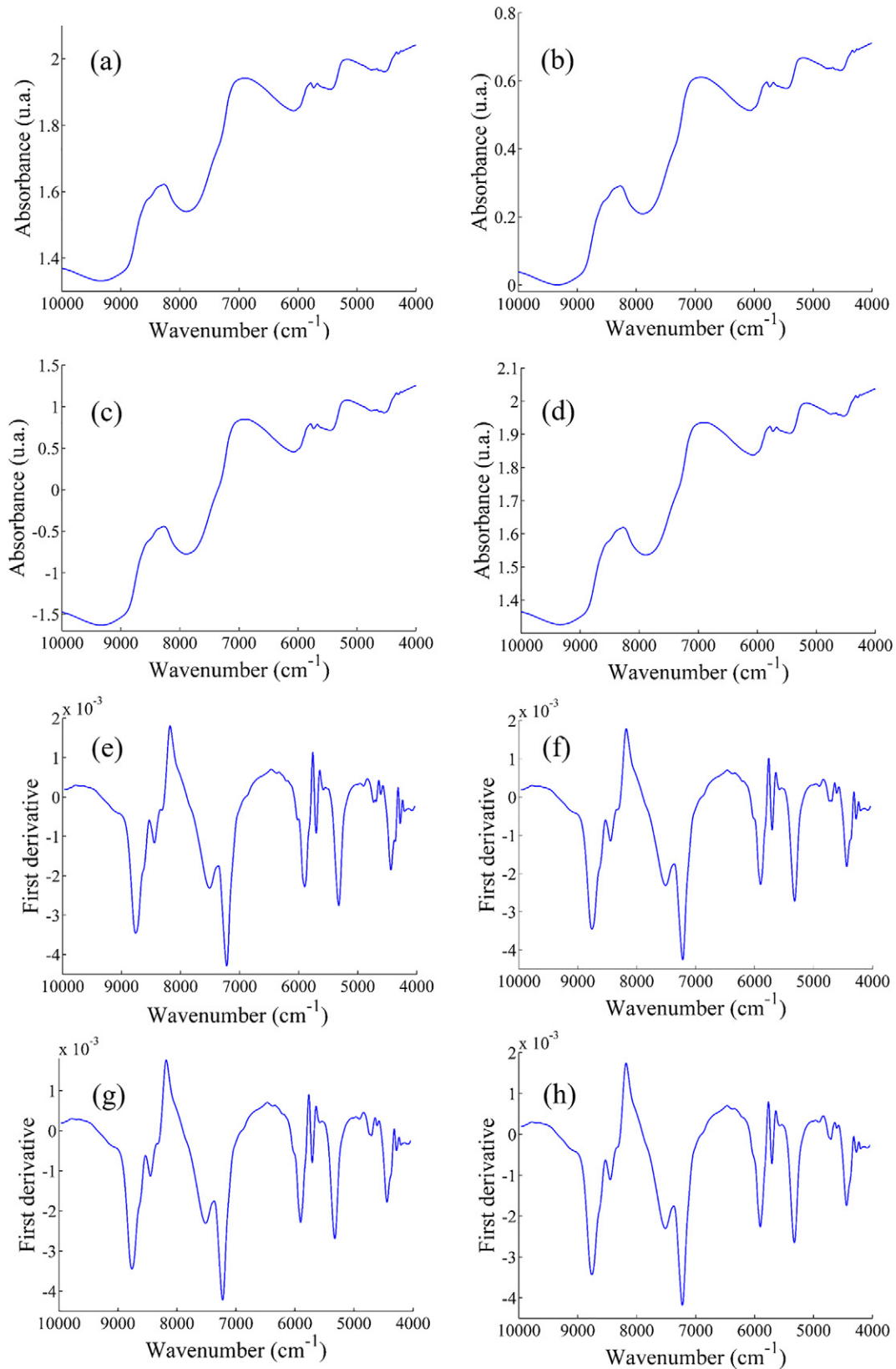 E-mail address: paulo.diniz@ufob.edu.br (P.H.G.D. Diniz).

Fig. 1. Mean NIR spectra of the 70 chicken hamburger samples: raw (a) and preprocessed spectra with base line correction (b), SNV (c), MSC (d) and first derivative Savitzky-Golay smoothing with a second-order polynomial and window sizes of 17 (e), 19 (f), 21 (g) and 23 (h) points.

fat content in natural products, pharmaceuticals and foodstuffs, including meat and meat products. The efficiency of several lipid extraction methods for quantification of fat in different meat products has been evaluated by Pérez-Palacios et al. [19]; however, these methodologies

have the disadvantage of being laborious and they use large amounts of sample and harmful solvents (chloroform, methanol, ether, etc.).

During the last decade, the importance of the development of new reliable methods of analysis for the quality control of meat products

Table 1
Best results for PLS modeling with different pre-processing methods for fat content determination in chicken hamburger samples.

Pre-processing method	LVs	Cross validation		Prediction			
		r_{CV}	RMSECV (mg kg^{-1})	RPD$_{Pred}$	r_{Pred}	RMSEP (mg kg^{-1})	REP (%)
Raw	11	0.79	3.35	1.19	0.50	3.86	18.7
Baseline correction	13	0.81	3.22	1.59	0.78	3.44	16.4
SNV	10	0.74	3.83	1.57	0.78	3.13	14.7
MSC	9	0.72	3.94	1.41	0.71	3.09	14.6
SG-1d-2o-17w	9	0.72	3.71	1.51	0.75	2.73	13.4
SG-1d-2o-19w	10	0.72	3.80	2.16	0.88	2.46	11.9
SG-1d-2o-21w	**10**	**0.74**	**3.73**	**2.31**	**0.90**	**2.33**	**11.2**
SG-1d-2o-23w	9	0.70	3.94	2.15	0.88	2.42	11.7

Best result for each multivariate calibration modeling (PLS, iPLS or iSPA-PLS) is indicated in bold.

like hamburgers has become evident. Vibrational spectroscopy such as Raman, Mid- and Near-Infrared Spectroscopy (MIR and NIR) has been highlighted because they are noninvasive and nondestructive methods, besides being sensible and fast. Furthermore, sample treatment is oftentimes not required.

Typical MIR and Raman spectra present peaks/bands at a specific frequency/wavenumber that are characteristics of functional groups of the sample constituents. Changes in the molecular dipole moment and in the polarizability during vibration are responsible for obtaining MIR and Raman spectra, respectively. This can be very useful for qualitative analysis, because the "fingerprints" of functional groups have narrow and intense peaks/bands in the region of 4000–400 cm^{-1}. For quantitative analysis, MIR has numerous applications, while Raman spectroscopy is more limited due to the need for complex pretreatment of the spectra. On the other hand, the peaks in the NIR region (1100–2500 nm or 9091–4000 cm^{-1}) are combinations and overtones of the sample functional groups and, for this reason, can be exhibited broadly and weakly [11,28]. Despite having frequently overlapping signals, NIR is still the most used technique, especially when coupled with suitable chemometric tools, and has been successfully applied as a routine analytic technique for meat quality control in different kinds of meats and meat products in terms of their fat content [1,3,4,20–22,24,27,29]. Additionally, the progress in instrumentation technology associated with the need for field-portable and easy-to-use devices has led to a current trend of miniaturization of various instruments. In such scenario, a handheld NIR spectrometer has been already used for meat quality control, in terms of investigating the content for fat, moisture and protein [30].

To achieve quantification of one or more analytes using NIR spectroscopy, suitable multivariate calibration techniques need to be used to relate the constituent concentration in a test sample to multiple measured instrumental responses (spectra). This procedure differs from univariate calibration, because in this case a single instrumental response is measured for each sample. In other words, in a more general multivariate calibration process it is possible to perform a rapid determination of mixture components (often with no prior separation, in the case of NIR spectroscopy) taking into account only the analyte of interest in complex samples while disregarding the concentrations of other components. This can be easily accomplished by using Partial Least Squares Regression (PLS), which works attributing weights to the X-variables, resulting in models that are easier to handle and interpret [13,14].

As typical NIR spectra have a large number of wavelengths for each sample, sometimes there is a redundancy of the recorded data due to the strong correlation over the different analytical channels. This affects both precision and accuracy of the results of the multivariate regression models such as PLS, which requires proper data preprocessing. In this context, selection of most informative spectral regions can significantly improve the performance of PLS regression, generating more stable models with superior interpretability, and fewer prediction errors. These improved predictions and parsimonious models are attained because the reduced set of variables diminishes consequently the number of interferences [5,8,10,17].

Other problems that generally affect typical NIR spectra are random noise and systematic variations in the baseline. These drawbacks can be overcame applying different preprocessing techniques, such as base line correction, standard normal variate transformation (SNV), multiplicative scatter correction (MSC), and Savitzky-Golay smoothing (SG). These mathematical pre-processing techniques remove the undesirable variations in the spectra that are unrelated to analyte concentration changes, providing better statistical performance by means of more parsimonious PLS models (generally with fewer latent variables) than those based on raw data [5,8].

The present work is focused on the development of an alternative analytical method based on near infrared spectroscopy and Successive Projections Algorithm for interval selection in PLS regression (iSPA-PLS) as used in the determination of fat content in commercial chicken hamburgers. The iSPA-PLS algorithm is an extension of SPA to select intervals of variables for use in PLS modeling, by combining the noise-reduction properties of PLS with the discard of non-informative variables in SPA [5,10]. For comparison purposes, full-spectrum PLS and the Interval PLS (iPLS) [17] were also used.

2. Materials and Methods

2.1. Samples Preparation

Chicken hamburgers were prepared in the laboratory with different fat content and minced chicken meat acquired in a local butcher shop in Bahía Blanca city, Buenos Aires, Province, Argentina. A stainless steel meat mincer machine was employed to mince the chicken fat and meat. Each one was passed 5 times in the mincer to ensure homogenization of the particle size. It is worth noting that the mincer was properly sanitized before the preparation of the chicken hamburger samples.

Seventy samples with a fat content ranging from 14.27 to 32.12 mg kg^{-1} were prepared in triplicate. We chose this range based on the upper limit recommended by the Argentinean Food Codex, which is 20% (w w^{-1}), taking into account that there might be possible adulterations with fat contents higher than that established in the regulation.

All samples were placed in a ring-shaped rubber support (sample holder) of 1.3 cm of internal diameter, 0.9 cm of height, and 1.5 g of capacity, in order to maintain the same dimensions.

2.2. Instrumentation and Software

#### 2.2.1. Near Infrared (NIR) Spectroscopic Analysis

Chicken hamburgers samples were analyzed in triplicate using a Thermo Scientific Spectrophotometer, Model Nicolet® IS50 FT-IR, in the reflectance mode and a spectral range between 4000 and

Table 2
Best results for iPLS modeling with different pre-processing methods for fat content determination in chicken hamburger samples.

Pre-processing method	LVs	Cross validation		Prediction			
		r_{CV}	RMSECV (mg kg^{-1})	RPD$_{Pred}$	r_{Pred}	RMSEP (mg kg^{-1})	REP (%)
Raw	6	0.76	3.54	1.45	0.72	3.09	14.9
Baseline correction	5	0.79	3.32	1.49	0.74	3.46	16.5
SNV	5	0.75	3.63	1.71	0.81	2.55	12.0
MSC	5	0.77	3.59	1.64	0.79	2.74	12.9
SG-1d-2o-17w	5	0.69	3.90	1.76	0.82	2.36	11.6
SG-1d-2o-19w	5	0.72	3.78	2.10	0.88	2.36	11.4
SG-1d-2o-21w	5	0.72	3.74	2.10	0.88	2.36	11.4
SG-1d-2o-23w	**5**	**0.73**	**3.73**	**2.11**	**0.88**	**2.34**	**11.3**

Best result for each multivariate calibration modeling (PLS, iPLS or iSPA-PLS) is indicated in bold.

Table 3
Best results for iSPA-PLS modeling with different pre-processing methods for fat content determination in chicken hamburger samples.

Pre-processing method	LVs	Best number of selected intervals	Cross validation		Prediction			
			r_{CV}	RMSECV (mg kg^{-1})	RPD $_{Pred}$	r_{Pred}	RMSEP (mg kg^{-1})	REP (%)
Raw	11	20/16	0.82	3.15	1.23	0.58	3.76	18.2
Baseline correction	13	5/4	0.81	3.22	1.60	0.77	3.37	16.1
SNV	5	5/4	0.75	3.63	1.70	0.81	2.55	12.0
MSC	9	10/4	0.78	3.51	1.67	0.80	2.51	11.8
SG-1d-2o-17w	9	20/17	0.75	3.52	1.70	0.81	2.45	12.0
SG-1d-2o-19w	**10**	**20/16**	**0.76**	**3.59**	**3.02**	**0.94**	**1.59**	**7.69**
SG-1d-2o-21w	10	10/7	0.76	3.51	2.90	0.94	1.83	8.81
SG-1d-2o-23w	9	10/5	0.75	3.64	3.02	0.94	1.78	8.56

Best result for each multivariate calibration modeling (PLS, iPLS or iSPA-PLS) is indicated in bold.
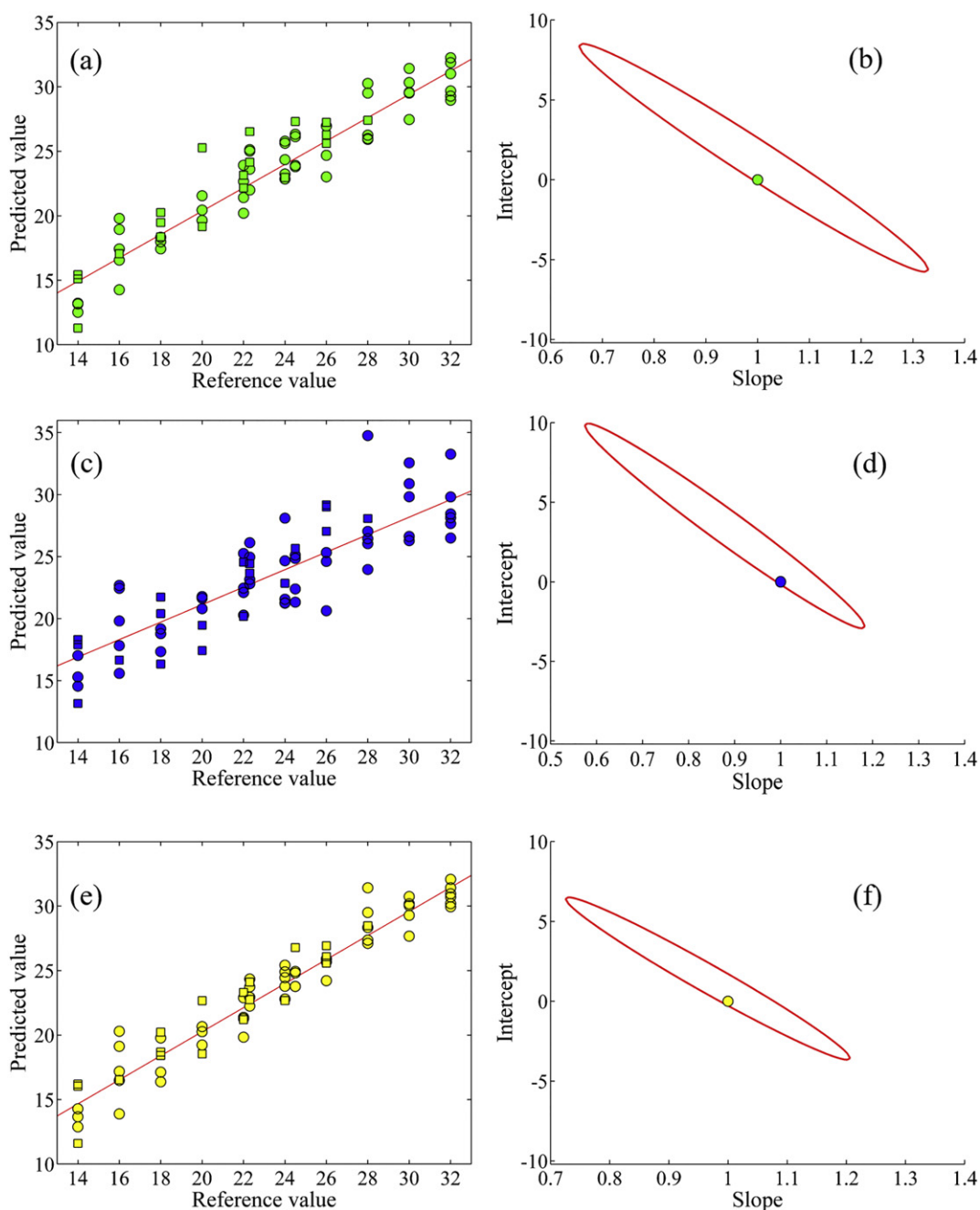
Fig. 2. Predicted vs reference plots for both calibration (circles) and prediction (squares) sets (a,c,e) and their respective elliptical joint confidence region plots containing the ideal theoretical point for the prediction set (b,d,f) for the best results obtained by PLS (a,b), iPLS (c,d) and iSPA-PLS (e,f), respectively.
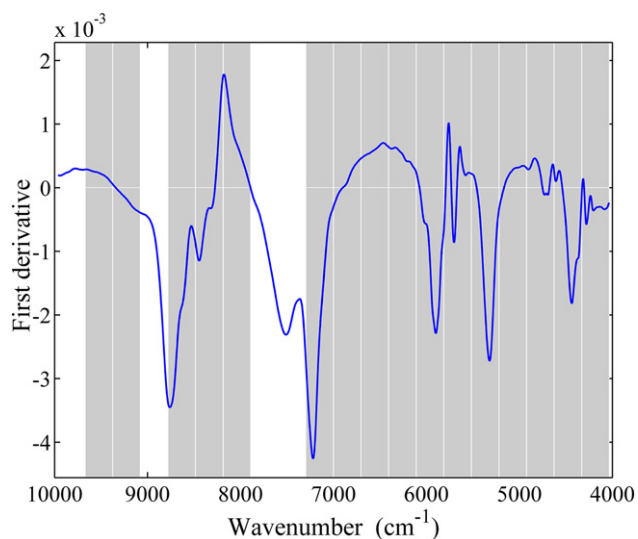
Fig. 3. Intervals of variables selected by the *i*SPA-PLS modeling constructed with NIR spectra preprocessed with first derivative Savitzky-Golay smoothing with a second-order polynomial and window size of 19 points.

10,000 cm^{-1}, with near-infrared reflectors (CaF$_2$/KBr) and detectors (InGaAs/KBr-DLaTGS). Reflectance spectrums were recorded using the integrated software, at 8 cm^{-1} spectral resolution and by integrating 32 scans. For each sample, an average spectrum was calculated from the triplicates registered for both upper and lower faces of the sample holder containing the chicken hamburgers. All measurements were carried out at room temperature (23 ± 1 °C) and used a reference internal standard of gold as the blank.

2.2.2. Chemometric Procedure

Initially, the dataset was organized in a matrix, where the samples are placed in rows and the registered spectra in columns. Since the spectra are noisy and exhibit systematic variations on the baseline, different preprocessing methods were applied to overcome these drawbacks: base line correction; standard normal variate transformation (SNV); multiplicative scatter correction (MSC); and first derivative Savitzky-Golay smoothing (SG) with a second-order polynomial and window sizes of 17, 19, 21 and 23 points.

From the dataset, 50 and 20 samples were selected for the calibration and prediction sets, respectively, by applying the Kennard–Stone (KS) uniform sampling algorithm that takes into account the X and y distances, simultaneously, in order to avoid extrapolation problems, and guarantees that the samples with the smallest and largest values of y are included in the calibration set. Then, three different Partial Least Squares (PLS) algorithms were evaluated: full spectrum PLS, the Interval PLS (*i*PLS) and the Successive Projections Algorithm for interval selection in PLS (*i*SPA-PLS). *i*PLS and *i*SPA-PLS were partitioned into 5, 10, 15 and 20 intervals. To optimize the number of PLS factors or latent variables (LV) to be included in the calibration set, the leave-one-out cross-validation technique was used, and its efficiency was evaluated according to the lowest root mean square error of cross-validation (RMSECV) and the highest correlation coefficient (*r*). The prediction was then only used for the final data evaluation and comparison of the multivariate calibration models. The predictive ability of the final models was evaluated in terms of the lowest values of both root mean square error of prediction (RMSEP), and the highest correlation coefficient (*r*). Relative error of prediction (REP) and ratio performance deviation (RPD) in the external prediction set were also evaluated for comparison of the performance of the models [5,7,9,10]. The elliptical joint confidence region (EJCR) test was applied in the prediction set
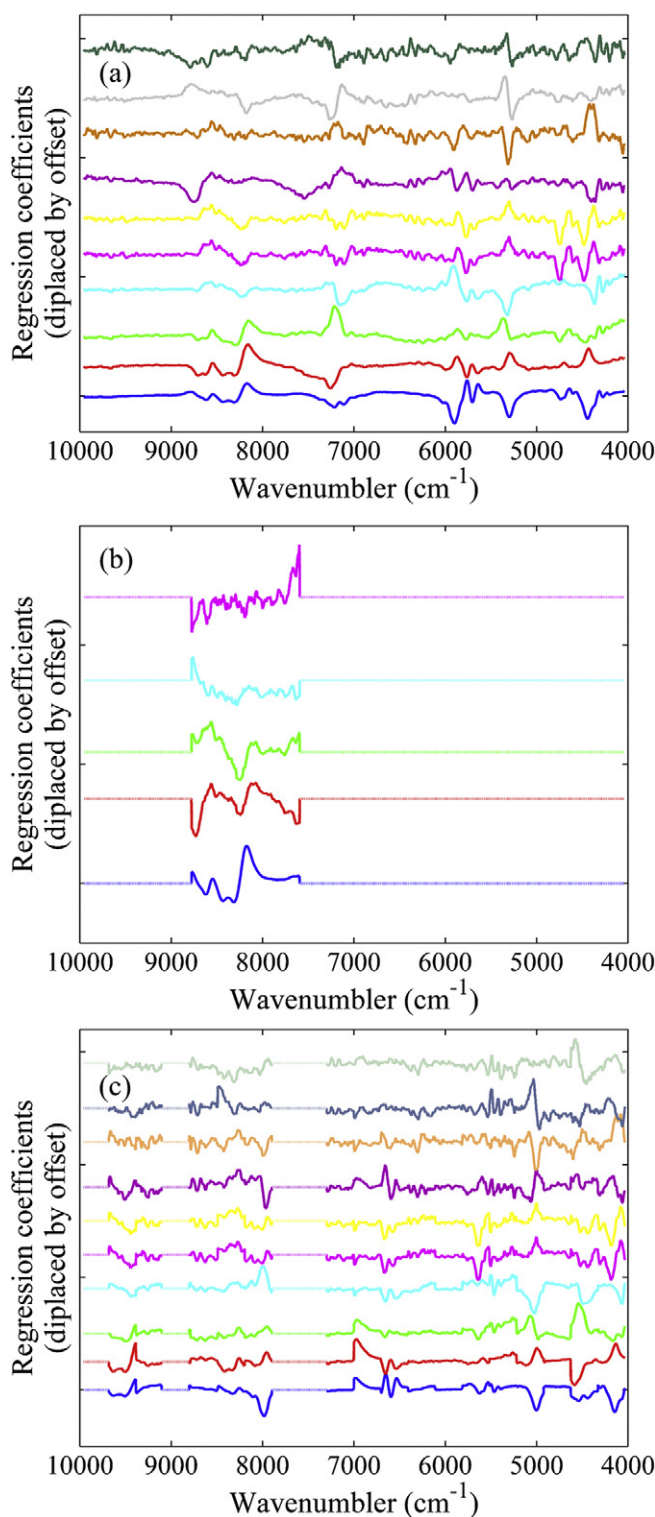

Fig. 4. Linear regression coefficients obtained for the best results of PLS (a), *i*PLS (b) and *i*SPA-PLS (c), respectively.

for all PLS models with different pre-processing methods in order to verify the accuracy of the constructed models, in which the results obtained by the chemometric modeling are compared with their respective reference values. For this purpose, an ordinary least squares (OLS) fitting was obtained, and the estimated intercept (a) and slope (b) were compared (with their ideal values of 0 and 1) using the EJCR test [6].

All chemometric procedures used throughout the work were implemented using Matlab® 2010a (Mathworks, USA).

3. Results and Discussion

3.1. Spectra Investigation and Pre-processing Procedures

Mean spectrum of the chicken hamburger samples with fat content ranging from 14.27–32.12 mg kg^{-1} is shown in Fig. 1a. As can be seen, intense spectral bands at 5150 cm^{-1} (a combination of O—H stretch and deformation) and 6900 cm^{-1} (the first overtone of O—H stretch vibration) have been mainly ascribed to water. The absorption band at 5900 cm^{-1} is associated with protein as amide. Other peaks at 8350 cm^{-1} (the second overtone of —CH stretch), 5800–5700 cm^{-1} (the first overtone of —CH stretch) and 4300–4260 cm^{-1} (combined —CH stretch and deformation band) correspond to fat content [31].

In order to eliminate noise and systematic variations on the baseline, different preprocessing methods were applied, as presented in Fig. 1b–h: (b) baseline correction, (c) SNV, (d) MSC, and first derivative Savitzky-Golay smoothing with a second-order polynomial and window sizes of (e) 17, (f) 19, (g) 21 and (h) 23 points. After pre-processing of the NIR spectra, PLS, iPLS and iSPA-PLS models were constructed. Their respective results are discussed in the next section.

3.2. Determination of Fat Content in Chicken Hamburgers

The reference values for the determination of fat content in chicken hamburgers were in the range of 14.27–32.12 mg kg^{-1}. These reference values were employed in the construction and prediction steps of PLS, iPLS and iSPA-PLS models using raw and pre-processed NIR spectra. Best results of the determinations of fat content in chicken hamburgers by using NIRS and PLS algorithms are summarized in Tables 1 to 3, respectively. Note that only the best results for the selection of intervals (partitioned into 5, 10, 15 and 20) in iPLS and iSPA-PLS are presented.

As indicated in Table 1, all pre-processing methods improved the result for PLS modeling when compared with raw spectra. The best performance was obtained by using first derivative Savitzky-Golay smoothing with a second-order polynomial and a window size of 21 points (PLS-SG-1d-2o-21w), achieving r_{CV} of 0.74, RMSECV of 3.73 mg kg^{-1}, r_{Pred} of 0.90, RMSEP of 2.33 mg kg^{-1}, REP of 11.2% mg kg^{-1} and RPD$_{Pred}$ of 2.31. To demonstrate the fit of the PLS-SG-1d-2o-21w model, a predicted vs reference plot for both calibration and prediction samples are shown in Fig. 2a. EJCR test (Fig. 2b) was then applied and demonstrates that the ellipse of the prediction model includes the theoretical ideal point, and therefore it presents no significant bias.

When iPLS was applied (Table 2), the REP values were slightly improved in relation to those obtained by full-spectrum PLS. As also observed for PLS modeling, the differing pre-processing methods presented a trend towards improving the results by using raw spectra, being the first derivative Savitzky-Golay smoothing with a second-order polynomial and window size of 23 points (iPLS-SG-1d-2o-23w). This was the best approach, achieving r_{CV} of 0.73, RMSECV of 3.73 mg kg^{-1}, r_{Pred} of 0.88, RMSEP of 2.34 mg kg^{-1}, REP of 11.3% mg kg^{-1} and RPD$_{Pred}$ of 2.11. These results associated with the predicted vs reference plot for both calibration and prediction samples for the iPLS-SG-1d-2o-23w model (Fig. 2c) confirms that the selection of one interval alone does not improve the result obtained for the full spectrum approach. Despite this, the EJCR test (Fig. 2d) demonstrated that the ellipse of the prediction model for iPLS-SG-1d-2o-23w presented no significant bias.

In the case of the iSPA-PLS models (Table 3), all approaches improved their respective results for PLS modeling. This occurred because the iSPA-PLS algorithm is an extension of SPA for selecting intervals of variables for use in PLS modeling, combining the noise-reduction properties of PLS with discarding non-informative variables in SPA.

Moreover, the adequate use of pre-processing methods of the NIR spectra enhanced the performance of the multivariate calibration techniques under study. Comparing the results, the best one was obtained with the first derivative Savitzky-Golay smoothing with a second-order polynomial and window size of 19 points (iSPA-PLS-SG-1d-2o-19w), achieving r_{CV} of 0.76, RMSECV of 3.59 mg kg^{-1}, r_{Pred} of 0.94, RMSEP of 1.59 mg kg^{-1}, REP of 7.69% mg kg^{-1} and RPD$_{Pred}$ of 3.02. The predicted vs reference plot for both calibration and prediction samples using iSPA-PLS-SG-1d-2o-19w revealed the best linear fitting when compared with PLS and iPLS. Moreover, when the EJCR test (Fig. 2f) was applied, the ellipse obtained for the iSPA-PLS-SG-1d-2o-19w model was more accurate and also included the ideal theoretical point. Note that only the iSPA-PLS-SG-1d-2o-19w model presented a RPD value higher than 3, as recommended and consensually accepted in the literature [7]. To achieve this result, the iSPA-PLS-SG-1d-2o-19w model selected 16 from 20 intervals (Fig. 3), which include the —OH, —NH and —CH band absorptions from water, protein and fat content, respectively. Therefore, the influence of the intrinsic variations of these parameters was included in the model, guaranteeing its stability. This agrees with the linear regression coefficients obtained for the best results obtained by PLS, iPLS and iSPA-PLS that exhibited higher intensities in the regions of the band absorptions related to water, protein and/or fat (Fig. 4). Comparatively, the linear regression coefficients obtained for iSPA-PLS generated a more parsimonious model with a higher predictive ability, as already confirmed by its figures of merit.

4. Conclusion

In this work, we demonstrated that the quality control of chicken hamburgers can be improved in terms of fat content by combining NIR spectroscopy and a suitable technique of selection of spectral intervals. For this, the Successive Projections Algorithm for interval selection in Partial Least Squares regression (iSPA-PLS) exhibited superior predictive performance when compared with full-spectrum PLS and iPLS. This was obtained by using NIR spectra preprocessed with first derivative Savitzky-Golay smoothing with a second-order polynomial and window size of 19 points, achieving a coefficient of correlation of 0.94, RMSEP of 1.59 mg kg^{-1}, REP of 7.69% and RPD of 3.02. The proposed methodology represents an excellent alternative to conventional Soxhlet extraction method, since it avoids waste generation, moreover without the use of either chemical reagents or solvents, which follows the primary principles of Green Chemistry. The new method was successfully applied to chicken hamburger analysis, and the results agreed with those of the reference values at a 95% confidence level, making it very attractive for routine analysis. However, a larger and more varied testing of meat types (e.g., bovine, swine, poultry) must be implemented to guarantee any generalization of the proposed methodology.

Compliance With Ethics Requirements

All authors declare that they have no conflict of interest. This article does not contain any studies with human or animal subjects.

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