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Prediction of the fatty acid composition of beef by near infrared transmittance spectroscopy

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Abstract

The intramuscular fat content and composition influence consumer selection of meat products. A study predicting the fatty acid (FA) profile of ground beef from the *Longissimus thoracis* of yearling bulls ($n = 100$) using near infrared transmittance spectroscopy (NIT) was conducted. The samples were scanned using an Infratec 1265 Meat Analyzer which operates in transmittance mode from 850 to 1050 nm. NIT technology was able to accurately predict (R^2_{CV} over 0.76) some prominent FAs such as C14:0, C16:0, C16:1*cis*9, C17:0, C18:1*cis*9 and C18:1*cis*11, and minor FAs like C13:0, C15:0, C17:1*cis*9 and C18:1*cis*13. When studying FA groups, NIT spectra were able to accurately predict saturated ($R^2_{CV} = 0.837$), branched ($R^2_{CV} = 0.701$) and monounsaturated ($R^2_{CV} = 0.852$) FAs. In addition, NIT spectra provided useful information on the contents of conjugated linoleic acids (CLA) in beef. These results show the potential of NIT technique as a rapid and easy tool to predict the major FAs in beef, especially those located in triglycerides.
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Keywords: NIT; Beef; *Longissimus thoracis*; Intramuscular fat; Fatty acid profile

1. Introduction

The quality of intramuscular fat of beef, in terms of content and fatty acid (FA) composition, is a key factor that influences its technological and sensory quality, mainly shelf-life (lipid and pigment oxidation) and flavour (Campo et al., 2003; Elmore, Mottram, Enser, & Wood, 1999; Vatansever et al., 2000; Wood et al., 2003). Furthermore, consumers have increased their interest in the fat composition of meat and meat products, as nutritional guidelines are recommending a lower total fat intake. More specifically, a lower saturated FA (SFA) intake and a higher polyunsaturated FA (PUFA) intake especially of $n-3$ FAs for an appropriate $n-6/n-3$ balance in order to avoid cardiovascular-type diseases (Connor, 1994; Mataix, Quiles, & Rodríguez, 2001). The consumption of beef in human diets also supply conjugated linoleic acids (CLA), which are a group of positional and geometrical isomers that are associated with important health-related benefits (Belury, 2003).

Intramuscular fat content and composition of ruminants depend on factors such as the genetic origin of the animals (Aldai et al., 2006a; Raes, De Smet, & Demeyer, 2001), feeding regime (Dannenberger, Nuernberg, Scollan, Ender, & Nuernberg, 2007; Gatellier, Mercier, Juin, & Renerre, 2005), age or live weight (Maltin et al., 1998; Okeudo & Moss, 2007) and influence the final quality of the product, which explains the increasing interest in defining the FA profile of meat from different production systems.

Typical methods used for FA determination are destructive and time-consuming. Moreover, they can be expensive and generate waste products of concern. The use of near infrared spectroscopy (NIRS) is increasing used in food analysis because it offers some advantages over conventional methods giving fast, non-destructive, clean and cost

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effective measurements (Osborne, Fearn, & Hindle, 1993). By constructing calibration models between NIRS spectra and chemical or quality tests, the NIRS technique can offer an accurate prediction of some complex quality attributes. More specifically, physico-chemical and organoleptic scores which allows delivery of real-time quality parameters before production is completed.

In meat, NIRS technology has been used to determine quality traits such as chemical composition (Alomar, Gallo, Castañeda, & Fuschslocher, 2003; Barlocco, Vadell, Ballesteros, Galietta, & Cozzolino, 2006; Isaksson, Nilsen, Togersen, Hammond, & Hildrum, 1996; Togersen, Isaksson, Nilsen, Bakker, & Hildrum, 1999), water holding capacity (Brondrum et al., 2000), and haem pigment content and colour (Leroy et al., 2003; Liu et al., 2003; Oliván, de la Roza, Martinez, & Mocha, 2001). Several studies also reported the potential of NIRS to predict Warner–Bratzler shear force and sensory tenderness in beef (Byrne, Downey, Troy, & Buckely, 1998; Hildrum, Nilsen, Mielnik, & Naes, 1994; Park, Chen, Hruschka, Shackelford, & Koohmaraie, 1998; Venel, Mullen, Downey, & Troy, 2001).

NIRS has also been applied to determine the total fat and FA composition in foods (without previous fat extraction or treatment of samples), such as in intact rapeseed (Sato, Uezono, Morishita, & Tetsuka, 1998) and edible vegetable oil (Chen & Chen, 1995). With respect to meat and meat products, it has been used for FA profile determination in pig fat (De Pedro, Garrido, Bares, Casillas, & Murray, 1992; García-Olmo, Garrido-Varo, & De Pedro, 2001), intact pork loins (González-Martín, González-Pérez, Álvarez-García, & González-Cabrera, 2005) and ground beef (Realini, Duckett, & Windham, 2004; Windham & Morrison, 1998).

The aim of the present work was to evaluate the potential of near infrared spectroscopy using transmittance (NIT) from 850 to 1050 nm to predict the FA composition (individual and main groups) in beef samples with a broad range of intramuscular fat contents.

2. Materials and methods

2.1. Meat samples

One hundred meat samples were obtained from the *Longissimus thoracis* (LT) muscle of yearling bulls of two local breeds from Northern Spain: "Asturiana de los Valles" (AV, $n = 75$) and "Asturiana de la Montaña" (AM, $n = 25$). Within the AV breed, animals had different double-muscling genotype, being homozygous (*mh*/*mh*, $n = 24$), heterozygous (*mh*/+, $n = 26$) and normal (+/+, $n = 25$). AM animals were normal (+/+) for this character, as this breed lacks the mutation responsible for double-muscling. At 24 h post-mortem, the LT steak of the eighth rib was dissected, vacuum packed and frozen at −80 °C for subsequent NIT and FA composition analyses. Before analysis, steaks were thawed overnight at 4 °C and minced with an electrical meat chopper (Moulinex 327, Spain).

2.2. Fatty acid analysis

Fatty acid composition was analyzed in duplicate by the method of Elmore et al. (1999), modified by Aldai, Murray, Nájera, Troy, and Osoro (2005) and validated by Aldai, Osoro, Barrón, and Nájera (2006b). Briefly, 1 g of muscle tissue was saponified in 6 mL 5 M KOH in methanol:water (50:50, v/v) at 60 °C for 1 h, and the extracted FAs were methylated using trimethylsilyl-diazomethane in methanol:toluene (2:1, v/v) at 40 °C for 10 min. FA methyl esters were identified according to the peak retention times and quantified according to the internal standard method (C21:0) added prior to saponification. The resulting data from the FA composition were previously published by Aldai, Nájera, Martinez, Celaya, and Osoro (2007) and were used as the "calibration data set" in this study.

2.3. Near infrared spectroscopy analysis

Near infrared spectroscopy analysis was performed using an Infratec 1265 Meat Analyzer (FOSS, Tecator AB, Höganäs, Sweden), which operates in transmittance mode from 850 to 1050 nm at 2 nm intervals. Samples (60 g) of minced meat were placed into a glass cup ($90 \times 90 \times 15$ mm) and scanned in duplicate. The spectrum of each sample was the average of five scan locations and was recorded as $\log 1/T$ (T = transmittance). The duplicate scans of each sample were examined for consistency and then averaged.

2.4. Statistical analysis

Spectral values were managed with the WinISI III software v. 1.61 (Intrasoft International, Port Matilda, PA, USA). The detection of anomalous spectra was accomplished using the Mahalanobis distance to the center of the population ($H \geqslant 3$). In addition, some samples were removed from the initial data set as concentration outliers, using the concentration residuals ($T > 2.5$).

Calibrations were performed using the Modified Partial Least Square (MPLS) method (Shenk & Westerhaus, 1993) and were assessed by cross-validation. To optimise the accuracy of calibrations, they were calculated on the crude spectra ($\log 1/T$) (NONE) or using a mathematical treatment based on the scatter correction Standard Normal Variate and Detrend (SNVD) (Barnes, Dhanoa, & Lister, 1989) and second derivative (2D). Then, two treatments were applied to the spectra: NONE (0, 0, 1, 1), and 2D-SNVD (2, 4, 4, 1). In brackets, the first number indicates the order of derivative, the second number is the gap in data points over which the derivative was calculated, the third number is the number of data points used in the first smoothing and the fourth refers to the number of data points over which the second smoothing was applied. The best treatment was selected for each constituent on the basis of the maximum values of the coefficients of determination in calibration (R^2) and cross-validation (R^2_{CV}). The

ratio of the standard deviation (SD) and the standard error of cross-validation (SECV), namely residual predictive value (RPD), was used to test the accuracy of the calibration models (Williams, 2001). When the RPD value was greater than two the prediction was considered good for analytical purposes, as reported by Barlocco et al. (2006).

3. Results and discussion

Table 1 summarises the descriptive statistics for the FA profile of the intramuscular fat in beef muscle samples included in NIT calibrations and determined by wet chemistry. FAs were organized as major (percentage over 1% of the total FA quantified) and minor (below 1%), being expressed in g/100 g muscle and mg/100 g muscle, respectively.

Table 1
Descriptive statistics for individual fatty acids in the intramuscular fat of beef samples included in near infrared transmittance calibrations

Fatty acid (FA)	Minimum	Maximum	Mean	SD
Major FAs (g/100 g muscle)				
C14:0	0.00	0.18	0.047	0.035
C16:0	0.12	1.40	0.497	0.272
C16:1*cis*9	0.00	0.15	0.040	0.027
C17:0	0.00	0.06	0.018	0.011
C18:0	0.06	0.58	0.224	0.104
C18:1*trans*	0.01	0.21	0.082	0.050
C18:1*cis*9	0.05	1.19	0.371	0.242
C18:1*cis*11	0.01	0.12	0.048	0.021
C18:2$n-6$	0.13	0.27	0.196	0.030
C20:4$n-6$	0.02	0.04	0.029	0.003
Minor FAs (mg/100 g muscle)				
C10:0	0.05	2.03	0.472	0.380
C12:0	0.12	3.66	1.048	0.709
C13:0	0.02	0.52	0.186	0.186
C14:1*cis*9	0.38	23.35	5.698	4.317
C15:0	1.28	23.57	6.935	4.530
*iso*C15:0	0.17	3.93	1.183	0.790
*anteiso*C15:0	0.44	5.54	1.986	1.155
*iso*C16:0	0.54	5.98	2.210	1.176
*iso*C17:0	1.42	7.97	3.730	1.537
C17:1*cis*9	1.06	32.50	10.146	7.087
*iso*C18:0	0.21	2.61	0.944	0.476
C18:1*cis*12	2.43	40.34	16.082	9.235
C18:1*cis*13	0.66	15.77	5.035	3.264
*cis*9,*trans*11-CLA	0.31	10.89	3.481	2.349
*trans*10,*cis*12-CLA	0.05	0.88	0.324	0.189
C18:3$n-6$	0.39	6.05	2.843	1.236
C18:3$n-3$	4.31	24.30	12.165	4.473
C19:0	0.32	6.35	1.978	1.427
C20:0	0.29	3.79	1.416	0.672
C20:2$n-6$	1.03	2.40	1.705	0.345
C20:3$n-6$	5.74	11.42	8.364	1.354
C20:3$n-3$	0.01	0.22	0.086	0.047
C20:5$n-3$	1.42	6.19	3.480	1.054
C22:0	0.04	0.57	0.214	0.130
C22:4$n-6$	2.94	5.94	4.282	0.691
C22:5$n-3$	3.95	11.07	7.482	1.395
C22:6$n-3$	0.21	0.97	0.583	0.194

SD: standard deviation.

Major FAs accounted for more than 93% of the total FAs quantified. Most of them showed a broad range of variability in the sample population, especially palmitic (C16:0) and oleic (C18:1*cis*9) acids which together account for around 50% of the total FAs studied. This broad range is important in order to obtain successful equations of calibration. Only two PUFAs had a major presence, linoleic (C18:2$n-6$; 12%) and arachidonic (C20:4$n-6$; 2%) acids. Within minor FAs, again, those with a wider range of concentration were in general those with a higher presence in meat: C14:1*cis*9, C15:0, C17:1*cis*9, C18:1*cis*12 and C18:3$n-3$.

When looking at the FA groups (Table 2), the sample set was found to encompass a wide range of SFAs and MUFAs (the main components of intramuscular fat), while the ranges of PUFAs were relatively limited. These variations in the SFAs and MUFAs were probably due to the high heterogeneity of total fat content of the meat samples included in this study (ranging from 0.562 to 4.409 g FAs/100 g muscle). However, PUFAs showed lower variability between samples (ranging from 0.20 to 0.36 g FAs/100 g muscle) probably because they are mainly located in membrane phospholipids, strictly controlled by a complex enzymatic system and relatively constant between individuals (Scollan et al., 2006).

Within the minor groups, branched fatty acids (BFAs) showed high variation between samples (3.43–26.64 mg/100 g). Higher levels of BFAs typically result when readily fermentable carbohydrate sources are available, causing an increase in propionate production (Wood, 1984). Then, synthesis of BFAs through carboxylation of propionil-CoA seems to be very likely (Duncan & Garton, 1978) as animals in our study received a high-barley concentrate (84% barley meal). However, as the diet was identical for all animals, differences in BFA absolute contents could be positively related to the intramuscular fat content, as previously found by Aldai et al. (2006a). With respect to CLAs, they were included in the NIT calibrations within

Table 2
Descriptive statistics for fatty acid groups in the intramuscular fat of beef samples included in near infrared transmittance calibrations

	Units	Minimum	Maximum	Mean	SD
SFA	g/100 g	0.19	2.31	0.795	0.447
BFA	mg/100 g	3.43	26.64	10.42	5.421
MUFA	g/100 g	0.11	1.76	0.586	0.360
PUFA	g/100 g	0.20	0.36	0.270	0.036
CLA	mg/100 g	0.54	10.97	3.855	2.508

SFA (saturated fatty acids) = C10:0 + C12:0 + C13:0 + C14:0 + C15:0 + C16:0 + C17:0 + C18:0 + C19:0 + C20:0 + C22:0; BFA (branched fatty acids) = *iso*C15:0 + *anteiso*C15:0 + *iso*C16:0 + *iso*C17:0 + *iso*C18:0; MUFA (monounsaturated fatty acids) = C14:1*cis*9 + C16:1*cis*9 + C17:1*cis*9 + C18:1*trans* + C18:1*cis*9 + C18:1*cis*11 + C18:1*cis*12 + C18:1*cis*13; PUFA (polyunsaturated fatty acids) = C18:2$n-6$ + *cis*9,*trans*11-CLA + *trans*10,*cis*12-CLA + C18:3$n-6$ + C18:3$n-3$ + C20:2$n-6$ + C20:3$n-6$ + C20:3$n-3$ + C20:4$n-6$ + C20:5$n-3$ + C22:4$n-6$ + C22:5$n-3$ + C22:6$n-3$; CLA (conjugated linoleic acids) = *cis*9,*trans*11-CLA + *trans*10,*cis*12-CLA; SD: standard deviation.

the PUFA group, but also were considered separately, due to their increasing importance from the consumer point of view as they have many purported roles in the prevention and possible treatment of several diseases (Belury, 2002; Ip, Masson-Welch, & Ip, 2003).

Fig. 1 reveals the average spectrum of the sample calibration set obtained in transmittance ($\log 1/T$) and its maximum and minimum spread. Crude spectra without pretreatment (Fig. 1a) showed a wide peak located from 930 to 1000 nm. It must be noticed, the large variation in absorbance between the maximum and minimum spectra, corresponding to the heterogeneity, in terms of fat content, of the meat sample set and probably to widely reported differences in collagen, colour and pigment content of beef from different genetic origins (AV and AM breeds or double-muscling character) (Aldai et al., 2006a; Clinquart, Hornick, Van Eenaeme, & Istasse, 1997; Oliván et al., 2004).

The application of a mathematical treatment to the NIT spectra based on the second derivative and scattering correction (2D-SNVD) (Fig. 1b) decreased the differences between maximum and minimum absorbances but revealed distinct peaks, mainly related with moisture (934–960 nm and 984–996 nm) and fat (962–968 nm), improving the prediction for most constituents studied. It is known that the use of derivative treatments not only reduces scattering effects but also increases the resolution of spectrum peaks (Davies & Grant, 1987). Furthermore, SNVD treatment improves NIRS predictions by reducing multicolinearity and the confounding effects of baseline shift and curvature (Dhanoa, Lister, & Baarnes, 1995).

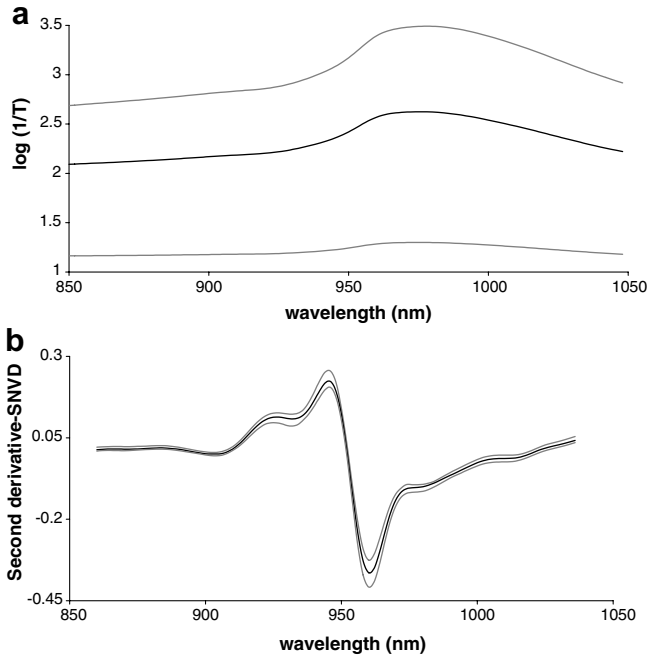

Fig. 1. Average near infrared transmittance spectrum (bold line) and its maximum and minimum spread (normal lines) of the sample calibration set for the mathematical treatments: (a) NONE (0,0,1,1) and (b) 2D-SNVD (2,4,4,1).

Separate NIT calibrations were obtained for individual FAs (Table 3) and groups (Table 4). As a whole, the best mathematical treatment in the majority of cases was the second derivative combined with SNVD treatment: 2D-SNVD (2,4,4,1). This is in accord with the report of Oliván, de la Roza, Mocha, and Martinez (2002) who found that the joint use of the second derivative and the SNVD treatment gave the best NIT calibrations for fat ($R^2_{CV} = 0.93$), moisture ($R^2_{CV} = 0.94$) and pigment contents ($R^2_{CV} = 0.91$) in beef. Also, Ding and Xu (1999) and Ding, Xu, and Chan (1999), showed that the SNVD correction improved the classification accuracy in minced beef and kangaroo. In the present work, when the best calibrations were obtained from the crude spectra (NONE treatment), the accuracy of predictions was, in general relatively low, with low coefficients of determination of cross-validation (R^2_{CV}), high SECVs and low RPDs.

Referring to NIT calibrations, the prediction values obtained for most individual SFAs were high (Table 3). Within major FAs, the best predictions were found for C14:0, C16:0 and C17:0, with R^2_{CV} over 0.80 and RPD over 2.2. Some minor SFAs, such as C13:0 and C15:0 were also highly predictable (RPD over 2.1). As a whole, the prediction of total SFAs (Table 4) was also positive, with $R^2_{CV} = 0.837$ and RPD > 2.4, as expected due to the fact that most of the FAs included in this group yielded good individual calibration equations (Table 3). In general, most researchers have described accurate NIRS calibrations for SFA group in meat, although comparisons are difficult due to the use of different equipment, wavelength ranges, sample preparation and chemical method for FAs analysis. Moreover, the present work is the first one where NIRS calibrations for meat FAs were calculated on a detailed FA profile including most minor FAs and using reference data expressed in absolute concentrations, while previous works expressed the data on a percentage basis, which makes comparisons between calibrations more difficult.

When using near infrared transmittance, De Pedro et al. (1992) and García-Olmo et al. (2001) obtained successful results for major SFAs (C16:0 and C18:0) in the subcutaneous fat of Iberian swine carcasses with R^2 values over 0.9. In ground beef and using reflectance, Realini et al. (2004) obtained good calibration statistics for total SFAs ($R^2_{validation} = 0.87$ and RPD = 2.6) and in particular for C18:0 ($R^2_{validation} = 0.91$, RPD = 2.6), for which we found a slightly lower prediction value ($R^2_{CV} = 0.737$, RPD = 1.9), in spite of being one of the major FAs in meat. In general our results are better than those reported for total SFAs on intact pork loin by González-Martín et al. (2005) using a remote reflectance optic probe, with $R^2_{CV} = 0.807$, SECV = 1.763 and SD = 2.62 (then RPD < 1.5) and those of Windham and Morrison (1998), who analyzed ground beef by NIR reflectance and obtained accurate predictions for total SFAs, with $R^2_{validation} = 0.77$ and RPD = 2.9, but not for individual SFAs (C14:0, C16:0 and C18:0) that were not accurately predicted with RPDs less than 2.0.

Table 3
Calibration and cross-validation statistics for determination of individual fatty acids in intramuscular fat by near infrared transmittance

Fatty acid (FA)	*N*	Mathematical treatment	Terms	SEC	R^2	SECV	R^2_{CV}
Major FAs							
C14:0	91	2D-SNVD	5	0.013	0.860	0.016	0.802
C16:0	92	2D-SNVD	5	0.105	0.851	0.115	0.831
C16:1*cis*9	92	2D-SNVD	6	0.011	0.829	0.013	0.790
C17:0	91	2D-SNVD	5	0.005	0.834	0.005	0.781
C18:0	93	2D-SNVD	5	0.051	0.764	0.055	0.737
C18:1*trans*	92	NONE	9	0.040	0.367	0.043	0.305
C18:1*cis*9	93	2D-SNVD	5	0.085	0.877	0.089	0.867
C18:1*cis*11	92	2D-SNVD	7	0.009	0.820	0.010	0.766
C18:2$n-6$	93	NONE	3	0.027	0.183	0.027	0.147
C20:4$n-6$	98	NONE	1	0.003	0.058	0.003	0.005
Minor FAs							
C10:0	90	2D-SNVD	6	0.167	0.806	0.200	0.755
C12:0	91	2D-SNVD	6	0.325	0.790	0.398	0.698
C13:0	93	2D-SNVD	5	0.066	0.662	0.079	0.569
C14:1*cis*9	88	2D-SNVD	6	2.001	0.785	2.466	0.731
C15:0	92	2D-SNVD	5	2.061	0.793	2.134	0.798
*iso*C15:0	98	2D-SNVD	6	0.407	0.735	0.446	0.690
*anteiso*C15:0	90	2D-SNVD	4	0.543	0.779	0.684	0.701
*iso*C16:0	94	2D-SNVD	7	0.619	0.723	0.658	0.699
*iso*C17:0	97	NONE	8	1.074	0.566	1.141	0.512
C17:1*cis*9	93	2D-SNVD	10	2.328	0.892	3.042	0.817
*iso*C18:0	94	NONE	11	0.294	0.619	0.301	0.602
C18:1*cis*12	92	NONE	9	4.717	0.739	4.930	0.716
C18:1*cis*13	93	2D-SNVD	9	1.350	0.829	1.523	0.797
*cis*9,*trans*11-CLA	97	2D-SNVD	3	1.462	0.613	1.543	0.582
*trans*10,*cis*12-CLA	96	NONE	2	0.180	0.090	0.202	0.079
C18:3$n-6$	97	NONE	11	0.990	0.358	1.116	0.192
C18:3$n-3$	94	NONE	10	2.564	0.671	2.696	0.637
C19:0	96	2D-SNVD	5	0.792	0.692	0.892	0.620
C20:0	98	2D-SNVD	4	0.378	0.684	0.405	0.645
C20:2$n-6$	91	NONE	10	0.286	0.315	0.307	0.204
C20:3$n-6$	96	2D-SNVD	1	1.314	0.058	1.342	0.029
C20:3$n-3$	89	2D-SNVD	8	0.039	0.328	0.051	0.098
C20:5$n-3$	91	NONE	1	1.059	0.009	1.053	0.004
C22:0	94	NONE	11	0.098	0.432	0.106	0.340
C22:4$n-6$	90	NONE	6	0.610	0.219	0.675	0.112
C22:5$n-3$	97	NONE	6	1.252	0.195	2.298	0.162
C22:6$n-3$	96	NONE	11	0.169	0.242	0.183	0.145

CLA: conjugated linoleic acids; *N*: number of samples in calibration; Terms: number of modified PLS factors used in calibration; SEC: standard error of calibration; R^2: coefficient of determination of calibration; SECV: standard error of cross-validation; R^2_{CV}: coefficient of determination of cross-validation.

Table 4
Calibration and cross-validation statistics for determination of fatty acid groups in intramuscular fat by near infrared transmittance

	N	Mathematical treatment	Terms	SEC	R^2	SECV	R^2_{CV}
SFA	93	2D-SNVD	5	0.168	0.859	0.182	0.837
BFA	96	2D-SNVD	4	2.645	0.747	2.907	0.701
MUFA	92	2D-SNVD	5	0.132	0.866	0.140	0.852
PUFA	93	NONE	3	0.031	0.252	0.033	0.244
CLA	96	NONE	7	1.612	0.587	1.613	0.586

SFA: saturated fatty acids; BFA: branched fatty acids; MUFA: monounsaturated fatty acids; PUFA: polyunsaturated fatty acids; CLA: conjugated linoleic acids; *N*: number of samples in calibration; Terms: number of modified PLS factors used in calibration; SEC: standard error of calibration; R^2: coefficient of determination of calibration; SECV: standard error of cross-validation; R^2_{CV}: coefficient of determination of cross-validation.

With regard to the NIRS prediction of BFAs, no information was found in the literature. Our study provided coefficients of determination in cross-validation (R^2_{CV}) of 0.7 for three individual BFAs (*iso*C15:0; *anteiso*C15:0 and *iso*C16:0) and when studying the BFA group, R^2 and R^2_{CV} were also over 0.7 in spite of its low presence in meat.

In the present work individual MUFAs were well predicted by NIR transmittance (Table 3), in that all R^2_{CV} values were over 0.7 except for C18:1*trans* which was relatively low ($R^2_{CV} = 0.367$). This was partly due to the coelution of major *trans* isomers (*trans*10 and *trans*11) and minor isomers (*trans*6–9 and *trans*12–14). Two com-

plementary GC (gas chromatography) temperature programs (Dugan et al., 2007) or a preparatory Ag^+-TLC (silver-ion thin-layer chromatography) separation followed by GC separation (Cruz-Hernández et al., 2004) are required for a more accurate C18:1*trans* isomer separation. Within the MUFAs, oleic acid (C18:1*cis*9) was the one with the best NIT prediction ($R^2_{CV} = 0.867$, RPD = 2.72), which agrees with previous results of González-Martín et al. (2005); Realini et al. (2004); Windham and Morrison (1998), as it is the most abundant MUFA (in the present study, it represented more that 20% of total FAs and more than 60% of total MUFAs). Its coefficient results for R^2_{CV} and RPD were similar to those of total MUFAs ($R^2_{CV} = 0.852$, RPD = 2.57). With lower contents in beef samples, C16:1*cis*9 and C18:1*cis*11 were also highly predictable ($R^2_{CV} > 0.766$ and RPD > 2), as well as some minor FAs, such as C17:1*cis*9 ($R^2_{CV} = 0.817$, RPD = 2.3) and C18:1*cis*13 ($R^2_{CV} = 0.797$, RPD = 2.1).

Individual PUFAs were the ones with the poorest predictions (Table 3). None of them reported R^2 values over 0.7, of which most were under 0.5. Linoleic acid (C18:2$n-6$) despite being one of the major FAs in meat, was not reliably predicted ($R^2_{CV} = 0.147$). With regards to linolenic acid (C18:3$n-3$), a major $n-3$ FA, it was better predicted ($R^2_{CV} = 0.637$) than C18:3$n-6$ ($R^2_{CV} = 0.192$). These results agree with previous findings of Windham and Morrison (1998), who reported even lower coefficients of validation for linoleic ($R^2_{validation} = 0.01$) and linolenic ($R^2_{validation} = 0.16$) acids in ground beef. Realini et al. (2004) did not find either a good calibration for linoleic, with a coefficient of prediction of 0.04. These authors, however, suggest that the failure to determine accurately these individual FAs could be related to similarities in their NIR absorption pattern, because different FAs have the same absorbing molecular group (–CH_2–), and also to the narrow standard deviation of the data sets. In the present study, the lack of spectral values from 1696 to 1724 nm where C18:2$n-6$ acid has its main absorption bands (Sato et al., 1998) could explain the poor prediction values for this FA.

Evaluation of individual PUFAs indicated that the CLA isomer *cis*9,*trans*11 had the best prediction ($R^2_{CV} = 0.582$, RPD = 1.52) in accord with the coefficients of the CLA group ($R^2_{CV} = 0.586$, RPD = 1.55). Recent research indicates that the major CLA isomers in beef are *cis*9,-*trans*11-CLA, and *trans*7,*cis*9-CLA and these coelute during GC analysis (Cruz-Hernández et al., 2004; Sehat et al., 1998).

The PUFA group (including CLAs) is the only one for which the crude NIT spectra reported better calibrations than the use of derivative and scattering corrections (Table 4) although in any case the calibration statistics met the requirements for analytical purposes. This could be due to the lack of information on the spectral region over 1200 nm related with FA molecules (Williams & Norris, 1987). But also to possible limited detection by NIT spectroscopy of the vibration bonds of those PUFAs included in structural phospholipids of the cell membranes (up to 80%, Dannenberger et al., 2004). Another reason could be, as mentioned earlier the small range of variability in PUFA content in our sample set when expressed in absolute concentrations (0.20–0.36 g/100 g of muscle). Nevertheless, González-Martín et al. (2005) reported good calibrations for the PUFA group ($R^2 = 0.858$) in meat, but their data were expressed on a percentage basis (2.62–9.91%). In our case, when expressing the PUFA content on a percentage basis, the data range stretched from a minimum of 6.60% to a maximum of 44.73%, resulting in a better coefficient of cross-validation ($R^2_{CV} = 0.614$) and residual predictive value (RPD = 1.5).

4. Conclusions

The results of this study show that NIT in the range 850–1050 nm provides accurate predictions of total SFA, BFA and MUFA contents in ground beef, as well as the amount of the more prominent individual FAs (C14:0, C16:0, C16:1*cis*9, C17:0, C18:1*cis*9, C18:1*cis*11) and others with lower concentrations (C13:0, C15:0, C17:1*cis*9 and C18:1*cis*13). Even though the prediction of the PUFA content did not meet the requirements for analytical purposes, the NIT spectra provided useful information on the contents of CLA (especially *cis*9,*trans*11 isomer). In summary, these results suggest that NIT technology could be used as a rapid and easy method to determine FAs in beef. More importantly, of those FAs (SFAs and MUFAs) at a high concentration in the triglycerides of the intramuscular fat.

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