Food Chemistry 403 (2023) 134403

Contents lists available at ScienceDirect

Food Chemistry

journal homepage: www.elsevier.com/locate/foodchem

Prediction accuracies of cheese-making traits using Fourier-transform infrared spectra in goat milk

Giorgia Stocco [a], Christos Dadousis [a], Michele Pazzola [b,*], Giuseppe M. Vacca [b], Maria L. Dettori [b], Elena Mariani [a], Claudio Cipolat-Gotet [a]

[a] Department of Veterinary Science, University of Parma, 43126 Parma, Italy
[b] Department of Veterinary Medicine, University of Sassari, 07100 Sassari, Italy

ARTICLE INFO

Keywords:
Goat
Cheese yield
Nutrient recovery
Farm
Infrared spectra

ABSTRACT

The objectives of this study were to explore the use of Fourier-transform infrared (FITR) spectroscopy on 458 goat milk samples for predicting cheese-making traits, and to test the effect of the farm variability on their prediction accuracy. Calibration equations were developed using a Bayesian approach with three different scenarios: i) a random cross-validation (CV) [80% calibration (CAL); 20% validation (VAL) set], ii) a stratified CV [(SCV), 13 farms used as CAL, and the remaining one as VAL set], and iii) a SCV where 20% of the goats randomly selected from the VAL farm were included in the CAL set (SCV_{80}). The best prediction performance was obtained for cheese yield solids, justifying for its practical application at population level. Overall results were similar to or outperformed those reported for bovine milk. Our results suggest considering specific procedures for calibration development to propose reliable tools applicable along the dairy goat chain.

1. Introduction

Cheese-making traits are fundamental to monitor the efficiency of dairy operations because they express the ratio between quantity and quality of the inputs and outputs of the cheese production. Among the pool of cheese-making traits, percentage cheese yield (%CY), the amount of cheese derived from a given amount of milk, is the most important economic trait for the cheese industry. The %CY traditionally relies on bulk milk measured at dairy industry level (Melilli et al., 2002), but for research purposes, it can also be assessed at individual animal level via laboratory model-cheese making procedures (Wedholm, Larsen, Lindmark-Mansson, Karlsson, & Andren 2006; Cipolat-Gotet, Cecchinato, Stocco, & Bittante, 2016). Those techniques offer the opportunity to collect a large number of samples and phenotypes by using a small quantity of milk in highly controlled and standardized procedure steps (e.g., cutting time, heating temperature), with the possibility to obtain also the recovery of milk nutrients (%REC) in the curd. Although few studies estimated the variability of measured %CY and %REC and their correlations with milk quality (Othmane, Carriedo, de la Fuente Crespo, & San Primitivo, 2002; Bittante, Cipolat-Gotet, & Cecchinato, 2013; Puledda et al., 2017), it is widely recognized that those traits do not solely depend upon fat and protein contents of milk, but also rely on the ability of the coagulum to retain the highest possible proportions of the available protein, fat, and water.

In caprine milk a limited number of studies investigated the farm variation in model cheese-making procedures applied on a large number of goats (Vacca et al., 2018; Paschino et al., 2020). However, cheese-making traits cannot be routinely measured, due to logistic issues mainly related to the onerousness of the sampling and high costs of analyses. To alleviate some of those difficulties, Fourier-transform infrared (FTIR) spectroscopy has been proposed as a useful tool for large-scale application to predict traits of interest from milk samples. In dairy cattle, FTIR spectroscopy has been used to investigate the suitability of the predicted %CY and %REC traits for their potential use at the dairy cattle population level (Ferragina, de los Campos, Vazquez, Cecchinato, & Bittante, 2015). Moreover, milk spectral data are

Abbreviations: %CY, cheese yield; %REC, recovery of milk nutrients; FTIR, Fourier-transform infrared spectroscopy; REP, repeatability; CV, Calibration-Validation procedures; SCV, Stratified Calibration-Validation procedure; CAL, calibration set; VAL, validation set; RMSE, root mean squared error; R2, coefficient of determination; SWIR, short wave infrared spectral region; MWIR, mid-infrared spectral region; MWIR1 and MWIR2, first and second mid-infrared spectral region; LWIR, long-infrared spectral region; MWIR-LWIR, transition between MWIR and LWIR.

* Corresponding author.
E-mail address: pazzola@uniss.it (M. Pazzola).

https://doi.org/10.1016/j.foodchem.2022.134403
Received 8 March 2022; Received in revised form 4 June 2022; Accepted 22 September 2022
Available online 30 September 2022

currently used in dairy cattle to develop calibration equations for a wide variety of traits which are, excluding milk components, phenotypes i) not directly measurable in milk, and mostly related to the environmental impact of the productive performances (i.e., methane emissions; Kandel et al., 2017), or to the animal status (i.e., energy balance; McParland et al., 2014); and ii) directly measurable in milk, as milk technological characteristics (i.e., milk coagulation properties; Visentin et al., 2015), with the underlying assumption that those traits are correlated with specific milk constituents, and therefore to specific chemical bonds (i.e., curd firmness is correlated with milk protein content, corresponding to the C═O, C—N, N—H and C—N signals of the spectrum). Currently, the use of FTIR spectroscopy is officially approved by the International Committee for Animal Recording only for the analysis of fat, protein, lactose and urea content in bovine milk (International Committee for Animal Recording [ICAR], 2021), but not for cheese-making traits.

In caprine milk, recent works have demonstrated the feasibility of FTIR spectroscopy to predict milk coagulation properties (Dadousis et al., 2021; Stocco et al., 2021), with prediction accuracies comparable to those reported in bovine (Chessa et al., 2014) and ovine milk (Ferragina et al., 2017). In particular, Dadousis et al. (2021) demonstrated the importance of considering the differences among farms in relation to coagulation traits during the development of the calibration models, to not incur in fictitious prediction accuracies (usually overestimated). Indeed, goat farming systems are highly different, and considerable variation for %CY and %REC traits attributed to single farms has been reported (Vacca et al., 2018).

Altogether, the economic importance of cheese-making traits in the dairy goat sector, the current limited knowledge on those milk technological traits, and the great worth of the information dwelling in the milk spectrum, justify the investigation of the use of FTIR spectroscopy in milk for the prediction of %CY and %REC traits at a wide-scale. Practically, the predicted cheese-making traits could be applied to different steps along the goat dairy chain, i.e., at the farm, breeding and dairy industry levels. To this purpose, the objectives of this study were to: i) investigate the potential use of FTIR spectroscopy for the prediction of % CY and %REC traits in goats, and ii) quantify the effect of the farm variability on the prediction accuracy of cheese-making traits using individual goat milk samples.

2. Materials and methods

2.1. Farm characteristics and milk sampling

The study involved 458 Sarda goats reared in 14 extensive and semi-extensive farms (F01-F14), distributed across the island of Sardinia (Italy). Farms characteristics were previously reported in Dadousis et al. (2021). Briefly, the extensive system (farms, N = 6) was characterized by family-managed farms, pasture feeding and natural mating; the semi-extensive system (farms, N = 8) was characterized by cultivated grasslands, control of estrus and kidding season. Goats were selected within animals officially registered in the flock books and enrolled in the milk recording system of associations of goat breeders on the basis of days in milk and parity, and to keep a good variability of milk quality. Individual milk samples (2 aliquots of 50 mL/goat) were collected during the afternoon milking (one sampling day for each farm), stored at 4 °C and analyzed within 24 h after collection.

2.2. Milk analysis and processing

For each milk sample, a FTIR spectrophotometer (MilkoScan FT6000; Foss, Hillerød, Denmark) was used to assess milk composition (percentage of fat, protein, lactose, and total solids; IDF 2013), and to collect the spectrum over the range from wavenumbers 5,011 to 925 × cm^{-1}. Spectra were stored as absorbance (A) using the transformation A = log(1/T), where T is the transmission. Two spectral acquisitions [absorbance (A) using the transformation A = log(1/T); T = transmission], were performed for each sample, and the results were averaged before data analysis (Fig. 1A).

The 9-mL milk cheese-making assessment (9-MilCA) proposed by Cipolat-Gotet et al. (2016) was used to measure %CY and %REC traits, with two replicates per each goat (2 × 9 mL) simultaneously processed, for a total of 916 observations. In brief, following the 9-MilCA, each milk replicate was: i) poured into a glass tube (9 mL), ii) weighted, iii) placed into the sample rack of the lactodynamograph instrument, iv) heated up to 35 °C for 15 min, v) and mixed with 0.2 mL of a rennet solution [Hansen Standard 215, with 80 ± 5 % chymosin and 20 ± 5 % pepsin; 215 international milk clotting units (IMCU)/mL (Pacovis Amrein AG, Bern, Switzerland); diluted to 1.2 % (wt/vol) in distilled water]. The sample rack was then moved to the lactodynamograph for a 30-min duration test at 35 °C. At the end of the analysis, coagulated milk samples were cut using a stainless steel spatula, and the rack was transferred to the heater for the 30 min curd-cooking phase at 55 °C. In the middle of the cooking phase, each sample was subjected to a second cut. At the end of the cooking phase, each glass tube was removed from the sample rack and the curd was separated from the whey. The curd was gently pressed and suspended above the whey for 30 min at room temperature in order to facilitate the draining. The obtained curd and whey were weighed using a precision scale. As the volume of whey produced from a single replicate/tube (about 7.5 mL) was not enough for the assessment of the chemical composition, the whey obtained from the two replicates of each milk sample was merged and analyzed for chemical composition by using an infrared spectrophotometer (MilkoScan FT2, Foss Electric) calibrated according to the reference IDF-ISO methods (IDF 22/ISO 7208 for fat; IDF 20/ISO 8968–1 for protein; IDF 198/ISO 22,662 for lactose). The weights of the milk, curd, and whey (in grams) and the chemical composition of milk and whey, allowed to estimate also curd composition. The choice of using the difference of milk-whey weight components was made because it guarantees a high repeatability of the calculated %CY and %REC traits (Cipolat-Gotet et al., 2016), the spectra can be collected from small amounts of milk and whey, and the predictions can be obtained very rapidly and inexpensively from many samples. Those characteristics are fundamental when a large number of samples has to be processed. The %CY traits consisted of $\%CY_{CURD}$, $\%CY_{SOLIDS}$ and $\%CY_{WATER}$, calculated as the ratio of the weight (g) of fresh curd, curd dry matter and water retained in curd, respectively, to the weight of the milk processed (g), and multiplied by 100. The %REC traits were $\%REC_{PROTEIN}$, $\%REC_{FAT}$ and $\%REC_{SOLIDS}$, calculated as the ratio of the weight (g) of the curd components (protein, fat and dry matter, respectively) to the same component of milk (g), and multiplied by 100. Moreover, the recovery of energy in the curd (**$\%REC_{ENERGY}$**) was calculated by estimating energy of milk and curd using an equation proposed by the Nutrient Requirements of Dairy Cattle (Nutrient Requirements of Dairy Cattle [NRC, 2001]), converted to MJ/kg and multiplied by 100.

2.3. Statistical analysis and FTIR spectra

2.3.1. Repeatability of cheese-making traits

Prior to the statistical analysis, all %CY and %REC values falling outside 3 standard deviations (SD) of the mean were excluded as outliers. To estimate the coefficient of repeatability (REP, expressed as percentage) of the %CY and %REC traits, the 2 replicates per goat were analyzed using a MIXED procedure (SAS Institute Inc., Cary, NC) that included the random effects of farm, animal, pendulum (measuring unit of the lactodynamograph instrument) and the residual. The REP for %CY and %REC traits was then calculated as the ratio of the sum of the variances of the random effects of farm, animal and pendulum to the total variance.

2.3.2. Editing of the spectra and chemometric model

Prior to spectra analysis, the absorbance values of every wavelength in the milk spectra of the analyzed milk samples were centered and

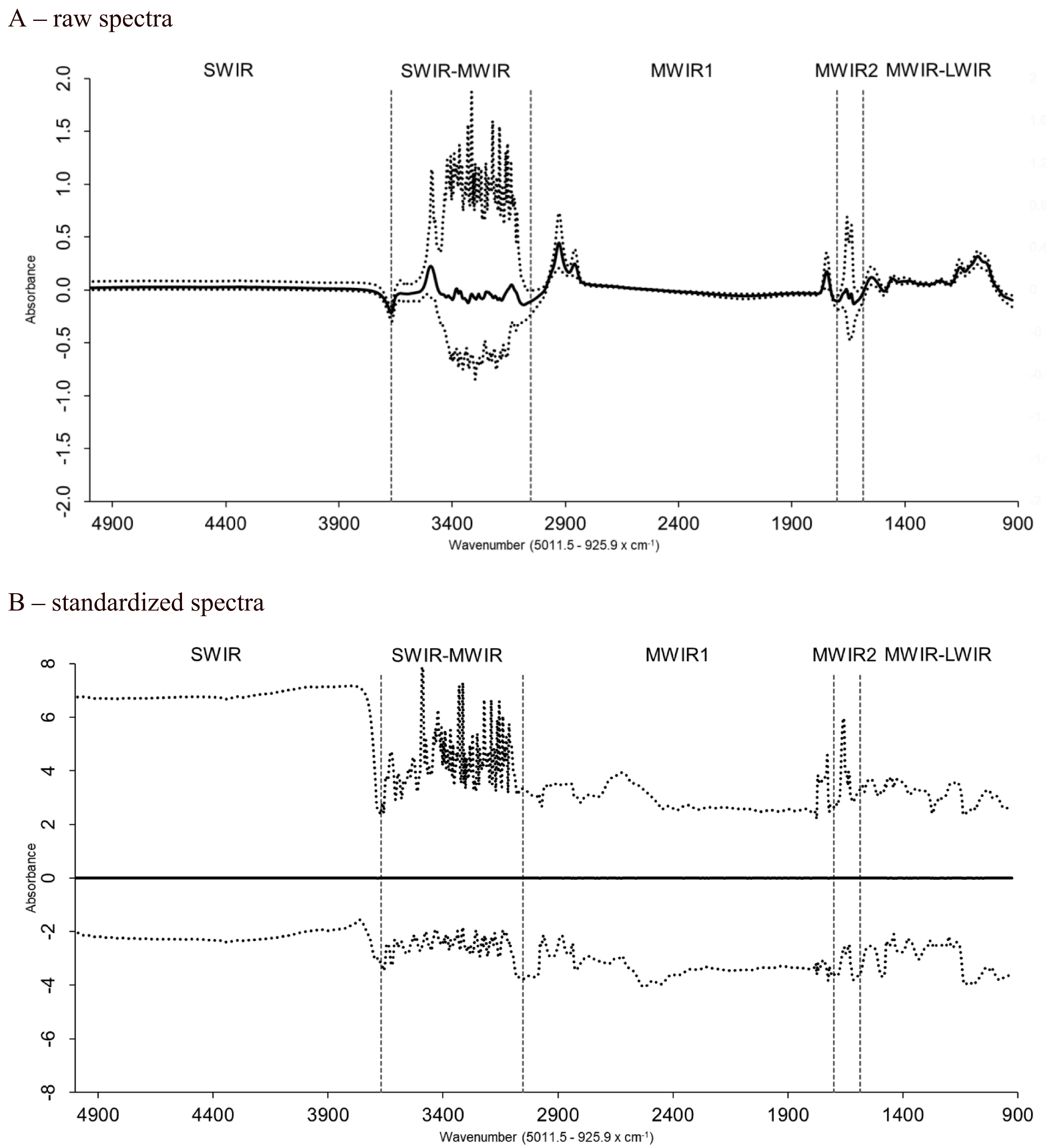


Fig. 1. Plots showing the absorbance of raw (a) and standardized (b) milk spectra (solid purple line represents the average, whereas the 2 dotted purple lines represent the maximum and the minimum of each wavelength, respectively).

standardized (Fig. 1B) to a null mean and a unit sample variance. Mahalanobis distances were calculated by the Mahalanobis function implemented in the R software (R Core Team, 2013) to detect outliers. All the spectra presented a distance value within the range of mean ± 3 SD, so no sample was discarded. The spectra were not subjected to any other mathematical pretreatment.

A Bayesian multiple linear regression was applied to predict the %CY and %REC traits. Each phenotype was regressed to 1,060 spectra simultaneously under the following model: $y = \mu + \sum_{j=1}^{1,060} x_{ij}\beta_j + e_i$, where μ is the overall mean, x_{ij} are the FTIR wavelengths, β_j are the regression coefficients and e_i the residual with *iid* $N(0, \sigma_e^2)$. The BayesB model in the *BGLR* R package was used (de los Campos, & Perez Rodriguez, 2015) as described in Ferragina et al. (2017).

2.3.3. Cross-validation and stratified cross-validation procedures

Prior to Calibration-Validation (CV) procedures, the two observations for %CY and %REC traits were averaged for each goat milk sample. The accuracy of the model and the prediction equation were assessed by a random CV and a Stratified CV (SCV) procedure. In the random CV, a calibration (CAL) set (80 % of the total records) was used to build the equation, and a validation (VAL) set (20 % of the total records) was used to test the model. The samples in the CAL-VAL sets were randomly assigned. To account for sample variability, the procedure was repeated 10 times for each trait and results were averaged over the 10 replicates.

Further, to quantify the farm effect on the predictive ability of the model, a SCV procedure was applied, predicting one farm at a time. Goat milk samples from 13 farms were used to build the equation (CAL set), and the remaining samples belonging to one farm were used to test the model (VAL set). The procedure was repeated 14 times, so that all farms were individually evaluated. In addition, to assess the importance of shared variability between CAL-VAL, another SCV, namely $\mathbf{SCV_{80}}$, was performed. In this procedure, 20 % of the goat milk samples from the farm to be validated was included in CAL, so that the VAL set consisted of the remaining 80 % of the goat milk samples of the same farm. The 20 % of the goats was randomly sampled and the procedure was repeated 10 times per farm. Results from the SCV procedure were averaged across the 14 farms, while in the case of the SCV_{80}, over the 10 replicates for each farm. The model performance was assessed by measures of root mean squared error (RMSE), coefficient of determination (R^2), in both CAL and VAL sets (R^2_{CAL} and R^2_{VAL}, respectively) and by residual predictive deviation (RPD), difference between measured and predicted values (bias), and the regression (measured vs predicted values) slope.

For each trait, the equation coefficients corresponding to each wavelength (N = 1,060), the Pearson correlations between each milk absorbance at a given wavelength, and the corresponding measured value of the trait were assessed. The results were plotted along the spectral range and divided into five IR regions as presented by Ferragina et al. (2017): short wave infrared (SWIR, often reported in literature as near-infrared), transition between SWIR and mid-infrared (SWIR-MWIR), first and second mid-infrared (MWIR1 and MWIR2, respectively) and transition between mid- and long-infrared (MWIR-LWIR).

3. Results and discussion

3.1. Informative wavelengths for predicting cheese-making traits

The use of Bayesian models for developing calibration equations from infrared milk spectra identifies the importance of wavelengths whose absorbance best predicts the objective trait, without the need to preselect any wavelength. The regression coefficients of BayesB represent a more informative way to test the calibrations respect to traditional methods such as partial least squares models. Their assessment includes their value at a specific wavelength, but also the value obtained from their multiplication with the absorbance at that wavelength of the spectrum. Furthermore, when comparing results to other studies, it is important to consider that the exact location and shape of the absorption bands along the spectrum may be affected by the experimental steps and lab conditions (i.e., pre-treatments of the samples, temperature, etc.), and the apparatus employed (Tiplady et al., 2019). In Fig. 2 are reported the calibration coefficients obtained using the BayesB method and Pearson correlations between the milk absorbance at a given wavelength and the predicted traits $\%CY_{CURD}$, $\%CY_{SOLIDS}$ and $\%REC_{SOLIDS}$, respectively. The pattern of correlations along the spectrum was comparable for the three cheese-making traits, with the highest rates in absolute value detected for $\%CY_{SOLIDS}$ in the regions of SWIR, MWIR1 and MWIR-LWIR, respectively. For the remaining %CY and %REC traits analyzed in this study, the pattern of correlations along the spectrum was found similar to that showed in Fig. 2, but with lower absolute values (data not shown). In agreement with Ferragina et al. (2015), the signals of the infrared spectrum were based on a relatively small number of wavelengths, with the highest regression coefficients being in the regions with moderate-high correlations.

3.1.1. The SWIR region

The SWIR extends from ~ 5,000 to ~ 3,673 wavenumbers × cm^{-1}. It exhibited positive and quite constant correlations along the entire spectrum interval, except for the wavenumbers from ~ 3,734 × cm^{-1}, and yet not consistent with any high regression coefficients for all cheese-making traits analyzed. This region of the spectrum is characterized by quite constant average values of the wavelengths. Moreover, even though O—H stretching produces a broad band occurring in the range between ~ 3,700 and ~ 3,600 wavenumbers × cm^{-1} (Stuart, 2004), the SWIR region is not known to contain any absorbance peak specific to a chemical bond in milk. Indeed, the correlations were quite constant and regression coefficients were low.

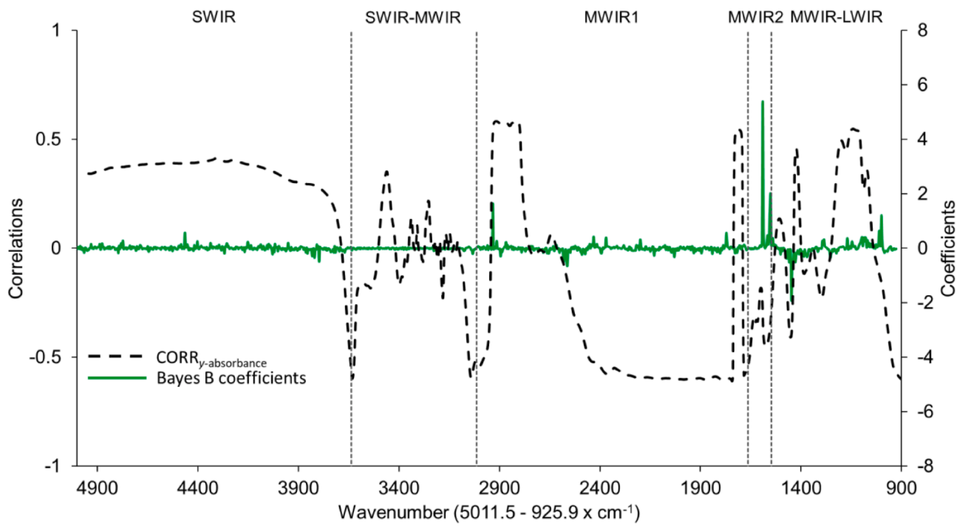
3.1.2. The SWIR-MWIR region

The SWIR-MWIR spans from ~ 3,669 to ~ 3,052 wavenumbers × cm^{-1}. Here, the N—H stretching is usually observed between ~ 3,400 and ~ 3,300 wavenumbers × cm^{-1}. This absorption is generally much sharper than O—H stretching and thus it can be more easily identified (Stuart, 2004). Most of the correlations in the SWIR-MWIR region, that include typical peaks related to water absorption (i.e., 3,490 and 3,280 wavenumbers × cm^{-1}), were close to zero (Fig. 1). However, for $\%CY_{SOLIDS}$, some wavelengths of this region had correlations higher than 0.50 (in absolute value) (Fig. 2B). The peaks related to the water absorption can significantly increase the variability of the spectrum, creating interference that could reduce the accuracy of calibrations. For this reason, the water absorption area is usually removed before the calibration development, even though this region contains significant chemical (i.e., N—H, C—N, N—O bonds) and genetic (i.e., heritability estimates > 5 % in Brown Swiss dairy cattle) information (Bittante, & Cecchinato, 2013; Tiplady et al., 2021). As aforementioned, the use of the variable selection BayesB model allows to select the most informative wavelengths as predictors (Ferragina et al., 2015). In our analyses, the signals (both in terms of correlation and regression coefficients) in the two water absorption regions of the infrared spectrum were close to zero (Fig. 2), in agreement with the results reported by Ferragina et al. (2017) for milk coagulation properties in sheep milk. Those authors observed opposite correlation patterns along the spectrum for gelation and curd firming time of sheep milk compared to our findings for $\%CY_{CURD}$, $\%CY_{SOLIDS}$ and $\%REC_{SOLIDS}$. However, this was expected given that the increase of gelation and curd firming time negatively affects the cheese-making process (Vacca, Stocco, Dettori, Bittante, & Pazzola, 2020). The regression coefficients in our analysis showed the largest variability for $\%REC_{FAT}$, with the wave at ~ 3,221 (wavenumber × cm^{-1}) revealing a high negative value (-0.51) of the average absorbance of the standardized spectrum (data not shown).

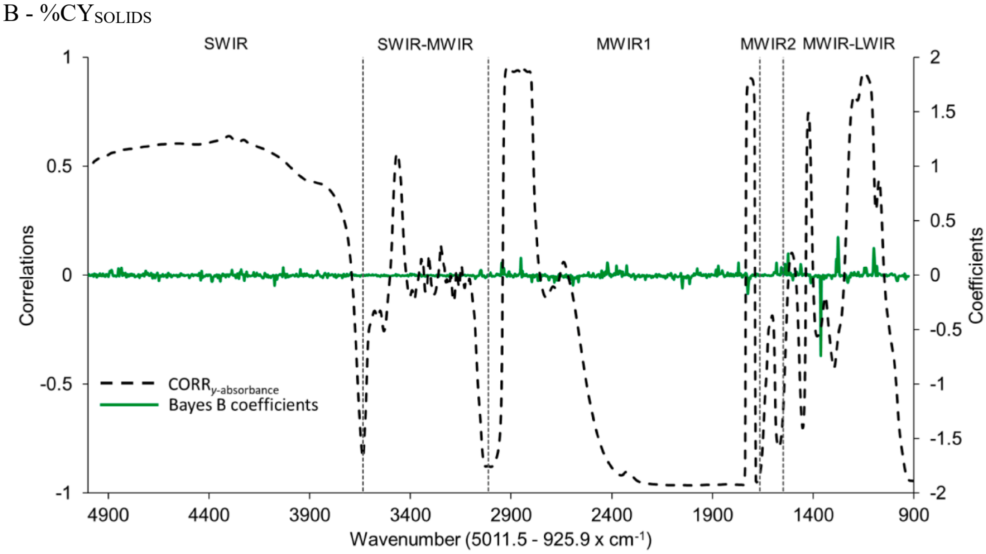
3.1.3. The MWIR-1 region

The MWIR-1 comprises the spectrum interval from ~ 3,048 to ~ 1,701 wavenumbers × cm^{-1}. This region is very informative for predicting milk composition, as it contains the major absorbance peaks for C—H, C═O, C—N, and N—H bonds. In the present study, MWIR-1 region was characterized by positive (from ~ 2,974 to ~ 2,800 wavenumbers × cm^{-1}) and negative values (from ~ 2,642 to ~ 1,774 wavenumbers × cm^{-1}) of correlation with cheese-making traits given in Fig. 2. In terms of regression coefficients of BayesB, the wavenumber at 2,932 wavenumbers × cm^{-1} for $\%CY_{CURD}$ showed a high value (1.65), where also the average absorbance of the standardized spectra was high (0.372). This wave is located close to the spectrum range known as "fat B" (2,870–2,778 wavenumbers × cm^{-1}), used to predict the fat content in milk (Kaylegian, Lynch, Fleming, & Barbano, 2009). Moreover, close to these wavelengths, Ferragina et al. (2017) reported several peaks (2,963 to 2,951 wavenumbers × cm^{-1}) to be important for the prediction of coagulation properties, and particularly for those traits related to the speed of gelation and firming of the curd. The MWIR-1 region includes also the spectral range usually referred as "fat A", which usually belongs to the interval between 1,786 and 1,725 wavenumbers × cm^{-1} (Kaylegian et al., 2009). In the present study, we found one of the highest and negative coefficients of BayesB (-0.17) for $\%CY_{SOLIDS}$ at the wavenumber 1,725 cm^{-1}. However, the average absorbance of the standardized spectra at that wavenumber is close to 0 (0.04), so its contribution in predicting this trait is low.

A - %CY_{CURD}



B - %CY_{SOLIDS}



C - %REC_{SOLIDS}

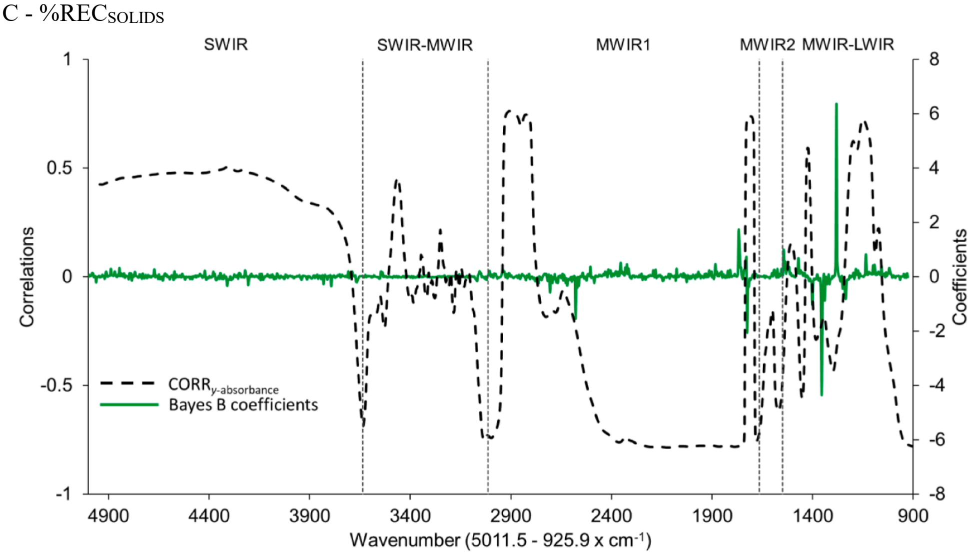


Fig. 2. Prediction equation coefficients obtained using the BayesB method (solid green line) and simple correlation coefficients (dashed black line) for the absorbance of each wavelength of the milk spectrum for the prediction of cheese-making traits (a, %CY_{CURD} = fresh cheese yield; b, %CY_{SOLIDS} = cheese yield in total solids; c, %REC_{SOLIDS} = recovery of total solids). Spectral regions are identified as short-wavelength infrared (SWIR), short and mid-wavelength infrared (SWIR-MWIR), MWIR-1, MWIR-2, and mid and long-wavelength infrared (MWIR-LWIR). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

3.1.4. The MWIR-2 region

The MWIR-2 represents the spectrum interval from ~ 1,698 to ~ 1,586 wavenumbers × cm^{-1}. Here, only negative Pearson correlations were found. For $\%CY_{CURD}$ a high regression coefficient was observed (5.40) at ~ 1,589 wavenumbers × cm^{-1} (Fig. 2A). This short region includes a typical peak related to water absorption (i.e., 1,645 wavenumbers × cm^{-1}), whose type of vibrational bond (H—O—H bending) causes very high absorbance of the radiation. Close to this spectral range, although not in the region MWIR-2, the wave at ~ 1,581 (wavenumbers × cm^{-1}) showed a high regression coefficient value (8.20) for $\%CY_{WATER}$ (data not shown). It is notable that the high regression coefficient associated with $\%CY_{CURD}$ was comprised within the water absorption area, and very close to that associated with $\%CY_{WATER}$. This could be explained by the fact that fresh curd is constituted for more than half of moisture. However, the MWIR-2 region of the milk spectrum contains other bond-related absorption peaks, beyond those due to water, such as those for acyclic and conjugated C—C, C═C, C═O, C—N, and N—H bonds, which in some instances are also heritable (Bittante, & Cecchinato, 2013).

3.1.5. The MWIR-LWIR region

The MWIR-LWIR is included within the spectrum interval from ~ 1,582 to ~ 930 wavenumbers × cm^{-1}. Positive and negative correlations were also observed here, but with larger values and with a more erratic trend compared to the other spectral regions. This spectrum range has been defined by Stuart (2004) as the fingerprint region, because it contains many bending and skeletal vibrations, for which small steric or electronic effects in the molecule result in large shifts in wavenumbers. This part of the spectrum harbors several peaks of absorbance associated to C—H, aromatic C═C, C—O, and N—O bonds (Stuart, 2004). In the specific case of milk, these bonds mainly correspond to carbohydrates and organic acids (Picque, Lefier, Grappin, & Corrieu, 1993). As a reflection of the importance of this region, here we observed the most informative wavelengths for predicting traits presented in Fig. 2. In particular, $\%CY_{SOLIDS}$ was associated with the highest five regression coefficients, one of them (1,524 wavenumbers × cm^{-1}) close to two important infrared signals for $\%CY_{CURD}$ (1,555 and 1,551 wavenumbers × cm^{-1}) and close to the spectrum range where absorbance is known to be associated with protein in bovine milk (1,547 to 1,478 wavenumber × cm^{-1}; Kaylegian et al., 2009). In those three wavelengths (1,555, 1,551 and 1,524, respectively), the average absorbance of the standardized spectra from our entire dataset was positive. Wavenumbers belonging to this region have also been associated with other traits in bovine milk, such as CH_4, 18:1 *trans*-10, 18:1 *trans*-11, 18:2 *cis*-9, *cis*-12 (Bittante, & Cipolat-Gotet, 2018) and $\%REC_{PROTEIN}$ (Ferragina et al., 2015).

3.2. Prediction accuracy of goat cheese-making traits

The dairy goat industry has been slowly evolving into a sustainable animal system, trying to implement changes in order to allow animal production to continue in an efficient and environmentally conscious manner. Monitoring and improving the efficiency of the dairy chain consists of several factors, among which data recording plays a major role. Moreover, large scale phenotyping by collecting high dimensional data at individual animal level has renewed the interest in dairy goats, while at the same time poses new challenges. Indeed, many innovative traits, such as the %CY-REC, are difficult to collect at the wide scale. Concurrently, actual knowledge on their genetic and biological background is lacking, and their relationships with other economically important traits of interest is not yet well-understood (Mrode et al., 2020). Cheese-making traits are by definition of major economic importance in the cheese industry, both for dairy producers and processors. The challenge is to develop a pipeline for a routine recording of the traits (i.e., large number of samples per day), at the population or herd level, and incorporate cheese traits in milk payment systems.

Descriptive statistics and prediction results of the CV procedure for %CY and %REC traits are presented in Table 1. Mean values were slightly higher respect to those previously reported for Sarda goat milk (Vacca et al., 2018) because of greater fat and water retention in the curd ($\%CY_{WATER}$ = 10.2 %; $\%REC_{FAT}$ = 85.9 %). Repeatability of %CY-%REC traits ranged from 93.2 % to 99.9 %. These values were higher compared to the REP values found in bovine (from 67.3 % to 99.9 %; Cipolat-Gotet et al., 2016), especially in the case of $\%CY_{WATER}$.

As regards to the prediction accuracy, the R^2_{VAL} and $RMSE_{VAL}$ from the CV procedure varied among traits. The R^2_{VAL} was lower and $RMSE_{VAL}$ was higher compared to the CAL set, even though data used in the calibration were characterized by much larger SD, except for $\%CY_{SOLIDS}$. In general, results in the VAL set were better than those previously reported for coagulation properties in individual caprine (Stocco et al., 2021) and ovine (Ferragina et al., 2017) milk samples. Particularly, the prediction of $\%CY_{SOLIDS}$ was very promising, with the R^2_{VAL} around 0.96, the low $RMSE_{VAL}$ (0.32 %) and the bias equal to 0.00 %. On the contrary, $\%REC_{FAT}$ was the only trait with a R^2_{VAL} below 0.50 (0.34) and presented the highest $RMSE_{VAL}$ (3.28 %) and the lowest bias (-0.27), even though this trait had the same REP as $\%CY_{SOLIDS}$. The SD of $RMSE_{VAL}$ for $\%CY_{SOLIDS}$ was the lowest among %CY traits, while that observed for $\%CY_{CURD}$ was the highest, as the trait is known to be affected also by the water retention in the curd ($\%CY_{WATER}$). We also tested the CV procedure for milk quality (i.e., composition and acidity; data not shown) in order to have a comparison within the dataset with traits usually predicted with FTIR spectroscopy (data not shown). It should be pointed out that results obtained for $\%CY_{SOLIDS}$ were comparable to those obtained for milk lactose and pH (data not shown).

Among %REC traits, $\%REC_{SOLIDS}$ had the highest R^2_{VAL} (0.81), the closest bias to 0 (-0.03 %) and a low $RMSE_{VAL}$ (1.86 %), similar to that found for $\%REC_{PROTEIN}$ (1.55 %). Indeed, $\%REC_{PROTEIN}$ had the lowest $RMSE_{VAL}$, probably because of its smallest variability (SD = 2.39 %) among %REC traits. Overall, the performances of prediction for %REC were lower than those obtained for %CY traits. In fact, while in the case of $\%CY_{CURD}$ and $\%CY_{SOLIDS}$ a predominant role of milk fat and casein is expected, the phenotypic correlation of $\%REC_{PROTEIN}$ and $\%REC_{FAT}$ with these two milk components is close to 0 (Bittante et al., 2013). Moreover, the $\%REC_{FAT}$ had a higher variability compared with $\%REC_{PROTEIN}$, and this probably contributed to the variability observed for the $\%REC_{SOLIDS}$ and $\%REC_{ENERGY}$. These last two traits are calculated from the protein, fat, and lactose content in milk. The milk components contributing to the variability of the cheese-making traits are not only those recovered in the curd (i.e., fat, protein in milk), but also those not participating to the curd formation (i.e., water, lactose), and the technological traits related to the coagulation process (i.e., curd firmness; Vacca et al., 2020), so that they can largely affect the validation performance of the %REC traits, in particular of $\%REC_{FAT}$. Indeed, the prediction statistics values between CAL and VAL set in the CV procedure were comparable within each %REC trait, except for $\%REC_{FAT}$, whose validation performance dropped (Table 1). However, it should be emphasized that for all the analyzed traits, the variance explained by the pendulum was close to 0, whereas that due to the animal was very high in agreement with results obtained by Vacca et al. (2018) in Sarda goats breed. In the present study, the percentage variance explained by the pendulum ranged from 0.002 % to 0.05 % respect to the total variance for cheese-making traits, while that explained by the individual animal was from to 44 % to 79 % (data not shown). This emphasizes the importance of understanding the genetic background of these traits and developing methods for indirect predictions on a wide-scale. Therefore, genetic parameters such as the heritability of measured %CY-%REC traits, or FTIR-predicted, have to be still estimated in dairy goats.

Overall, the fitting statistics of the CV scenario were comparable and, in some cases, overreached those reported for cheese-making traits in bovine milk. In the CV procedure, the prediction models for cheese-making traits had slopes between 0.94 and 1.03. Williams (2007) reported that when a slope deviates greatly from 1 (e.g., <0.85 and 1.15 or

Table 1
Descriptive statistics, repeatability (REP) of cheese-making traits[1] obtained by 9-MilCA and results (Mean ± SD) from the Cross-Validation procedure using infrared spectra from individual goat milk samples.

	Cheese yields (%CY)			Milk nutrients recovery in the curd (%REC)			
	$\%CY_{CURD}$	$\%CY_{SOLIDS}$	$\%CY_{WATER}$	$\%REC_{PROTEIN}$	$\%REC_{FAT}$	$\%REC_{SOLIDS}$	$\%REC_{ENERGY}$
Descriptive Statistics							
N	916	916	896	885	880	905	904
Mean ± SD	19.2 ± 3.27	8.91 ± 1.48	10.2 ± 2.28	81.1 ± 2.39	85.9 ± 4.07	60.4 ± 4.21	70.5 ± 4.12
Interval[2]	11.78–30.25	4.99–14.09	4.88–16.78	75.05–87.67	75.08–94.69	50.14–71.13	58.17–79.65
REP[3]	95.0	99.9	93.2	99.4	99.9	99.2	99.5
Prediction Statistics							
Cross-Validation							
N_{CAL}	366	366	362	355	352	362	362
R^2_{CAL}	0.78 ± 0.06	0.97 ± 0.01	0.67 ± 0.04	0.66 ± 0.12	0.50 ± 0.03	0.85 ± 0.04	0.75 ± 0.08
$RMSE_{CAL}$	1.52 ± 0.16	0.30 ± 0.05	1.30 ± 0.08	1.39 ± 0.22	2.91 ± 0.08	1.66 ± 0.20	2.07 ± 0.32
SD_{VAL}	3.34 ± 0.26	1.47 ± 0.14	2.36 ± 0.15	2.47 ± 0.17	4.00 ± 0.13	4.25 ± 0.25	4.17 ± 0.25
R^2_{VAL}	0.77 ± 0.06	0.96 ± 0.01	0.64 ± 0.09	0.62 ± 0.13	0.34 ± 0.10	0.81 ± 0.05	0.70 ± 0.07
$RMSE_{VAL}$	1.63 ± 0.23	0.32 ± 0.05	1.43 ± 0.18	1.55 ± 0.24	3.28 ± 0.20	1.86 ± 0.30	2.28 ± 0.32
RPD[4]	2.07 ± 0.27	4.71 ± 0.82	1.67 ± 0.22	1.62 ± 0.23	1.23 ± 0.08	2.34 ± 0.37	1.85 ± 0.21
Bias	0.00 ± 0.25	0.00 ± 0.02	0.02 ± 0.22	0.04 ± 0.27	−0.27 ± 0.39	−0.03 ± 0.16	0.09 ± 0.26
Slope	1.03 ± 0.08	0.99 ± 0.09	0.94 ± 0.12	0.95 ± 0.15	0.95 ± 0.15	1.01 ± 0.08	1.02 ± 0.10

[1] Cheese yields (%CY; weight of fresh curd, curd solids, and curd water as percentage of weight of milk processed); milk nutrients recovery in the curd (%REC; weight of the curd component (protein, fat, total solids, energy) to the same component in milk, multiplied by 100);
[2] Interval, minimum and maximum of observed values;
[3] Repeatability (REP), % = $\frac{\sigma^2_{Farm} + \sigma^2_{Animal} + \sigma^2_{Pendulum}}{\sigma^2_{Farm} + \sigma^2_{Animal} + \sigma^2_{Pendulum} + \sigma^2_e} \times 100$;
[4] RPD, Residual predictive deviation.

greater) results in an unstable calibration, while a prediction equation with a slope between 0.95 and 1.05 is more reliable. Ferragina et al. (2015), using similar statistical model and CV structure in Brown Swiss milk samples, found R^2_{VAL} of 0.71, 0.65, and 0.28, and $RMSE_{VAL}$ values of 1.03, 1.44, and 3.13, for $\%CY_{CURD}$, $\%REC_{PROTEIN}$ and $\%REC_{FAT}$, respectively. Bittante and Cipolat-Gotet (2018), using the same dataset, reported values of 0.79 and 0.43 for R^2_{VAL} and RMSE, respectively, predicting $\%CY_{SOLIDS}$. Moreover, El Jabri et al. (2019) compared a Bayesian linear regression with partial least squares regression on milk FTIR to predict cheese-making traits in milk from Montbéliarde cows, with best prediction models achieving R^2_{VAL} of 0.85–0.91 for $\%CY_{CURD}$ and $\%CY_{SOLIDS}$, respectively. Respect to our study, the water regions of the milk spectrum were removed prior the partial least squares model. Prediction of $\%CY_{CURD}$ from milk of Sarda sheep has been reported in Cellesi et al. (2019). In that study the authors compared different data pretreatments on milk spectra, and reported R^2 between observed and model predicted values from 0.60 to 0.66, and RMSE from 4.81 to 5.19 %. The high RMSE was probably due to high value of $\%CY_{CURD}$ (average = 35.8 %; SD = 8.20 %), as a consequence of the use of the centrifuge to separate the curd from the whey. That specific lab procedure, although reducing the processing time of milk samples, provides estimates of cheese-making far from mimicking a routine dairy plant cheese procedure.

3.3. Effect of farm variability on the prediction accuracy of cheese-making traits

It is widely recognized that among the factors influencing the reliability of FTIR predictions, the goodness (repeatability and accuracy) of the reference values has to be taken into account. This is certainly acceptable for the major milk components, which can be directly predicted from the individual wavelengths of the milk spectrum. In opposite, the variability of the indirectly predicted traits, as %CY and %REC traits here investigated, can be affected by several factors involved in the cheese-making process (i.e., curd firming and syneresis) that are quite difficult to detect through infrared spectroscopy. Moreover, reliability of FTIR predictions for indirect traits can be related to factors associated with the variability of the data (i.e., variability among animals, farms, breeds etc.) that cannot be controlled by standard statistical procedures such as CV. Despite those problems, milk spectra derived from FTIR spectroscopy have been proposed as a useful tool able to discriminate species (Nicolaou, Xu, & Goodacre, 2010), breeds (Salleh et al., 2019) and feeding systems (Valenti et al., 2013).

As shown by Wang and Bovenhuis (2019) using infrared milk spectra to predict traits related to methane emission in dairy cattle, a CV can overestimate the accuracy of the predictions, while SCV provides a more realistic view. The reduction of the RPD for all the cheese-making traits from the CV to the SCV confirmed the need of exploring other CV procedures (Table 1). Farms included in this study were characterized by extensive and semi-extensive goat farming management where, in general, higher variability is expected compared to intensive farming systems.

Table 2 summarizes the fitting statistics of the SCV procedure for %CY-%REC traits, while in Fig. 3 are plotted the R^2_{VAL} values obtained from the SCV_{80} procedure. On average, the prediction statistics of $\%CY_{SOLIDS}$ for SCV (R^2_{VAL} = 0.93 and bias = 0.03 %, respectively) confirmed the results observed for the CV, followed by those observed for $\%REC_{SOLIDS}$ and $\%REC_{PROTEIN}$ (R^2_{VAL} = 0.70 and 0.64, respectively). Interestingly, comparable results were found for $\%REC_{PROTEIN}$ between CV and SCV scenarios. On the contrary, the highest decrease in R^2_{VAL} up to 50 % was found for $\%CY_{WATER}$ and $\%REC_{FAT}$. Particularly, although the average of bias for $\%REC_{FAT}$ among farms was lower respect to the CV, the SD was very high (2.04 %). Moreover, the prediction models for $\%CY_{WATER}$ and $\%REC_{FAT}$ had slopes of 0.74 and 0.68 and therefore may have unstable calibrations (Williams, 2007).

The ranking of the traits in terms of performances of prediction was not the same of that observed for the CV. However, scatter plots of predicted versus measured values for the best predicted traits ($\%CY_{CURD}$, $\%CY_{SOLIDS}$ and $\%REC_{SOLIDS}$) obtained for CV and SCV resulted similar (Fig. 1S) while they were less comparable for those traits presenting lower performance of prediction. Those findings are also due to the relationships between traits and factors affecting their variability (es. individual farms and goats). For example, the variability of $\%REC_{PROTEIN}$ is more related to individual goats instead of farms (SD_{VAL} average for CV and SCV were 2.47 and 2.14, respectively). This is also supported by observing the R^2_{VAL} interval for $\%REC_{PROTEIN}$, the lowest excluding $\%CY_{SOLIDS}$ and $\%REC_{FAT}$ that presented the greatest and worst prediction statistics, respectively, but also examining the within-farm $\%REC_{PROTEIN}$ variability in the Fig. 3. Moreover, Pazzola et al. (2019), analyzing goat milk from different breeds, have shown that $\%REC_{PROTEIN}$ was affected

Table 2
Prediction statistics (Mean ± SD) of cheese making-traits[1] obtained by 9-MilCA from the Stratified Cross-Validation procedure using infrared spectra from individual goat milk samples.

Stratified Cross-Validation[2]	Cheese yields (%CY)			Milk nutrients recovery in the curd (%REC)			
	$\%CY_{CURD}$	$\%CY_{SOLIDS}$	$\%CY_{WATER}$	$\%REC_{PROTEIN}$	$\%REC_{FAT}$	$\%REC_{SOLIDS}$	$\%REC_{ENERGY}$
SD_{VAL}	2.34 ± 0.53	1.23 ± 0.34	1.59 ± 0.35	2.14 ± 0.30	3.33 ± 0.67	3.46 ± 0.75	3.49 ± 0.63
R^2_{VAL}	0.63 ± 0.12	0.93 ± 0.05	0.37 ± 0.17	0.64 ± 0.12	0.15 ± 0.13	0.70 ± 0.18	0.57 ± 0.21
$R^{2\,interval}_{VAL}$	0.38–0.97	0.81–0.97	0.08–0.63	0.46–0.85	0.00–0.36	0.23–0.90	0.24–0.86
$RMSE_{VAL}$	1.79 ± 0.52	0.40 ± 0.15	1.61 ± 0.44	1.79 ± 0.49	3.60 ± 0.85	2.06 ± 0.47	2.61 ± 0.46
$RMSE^{interval}_{VAL}$	0.97–2.75	0.18–0.68	0.88–2.38	0.99–2.48	2.44–4.18	1.51–3.38	1.73–3.46
RPD[3]	1.39 ± 0.43	3.39 ± 1.18	1.03 ± 0.27	1.28 ± 0.36	0.94 ± 0.16	1.74 ± 0.47	1.37 ± 0.33
Bias	0.05 ± 1.15	0.03 ± 0.25	0.05 ± 0.98	0.12 ± 1.27	0.07 ± 2.04	0.04 ± 0.95	−0.21 ± 1.34
Slope	0.91 ± 0.18	0.96 ± 0.09	0.74 ± 0.24	0.97 ± 0.21	0.68 ± 0.42	0.99 ± 0.20	0.92 ± 0.28

[1] Cheese yields (%CY; weight of fresh curd, curd solids, and curd water as percentage of weight of milk processed); milk nutrients recovery in the curd (%REC; weight of the curd component (protein, fat, total solids, energy) to the same component in milk, multiplied by 100);
[2] For R^2_{VAL} and $RMSE^2_{VAL}$ of Stratified Cross-Validation also interval of 14 farms cross validations was included;
[3] RPD, Residual predictive deviation.

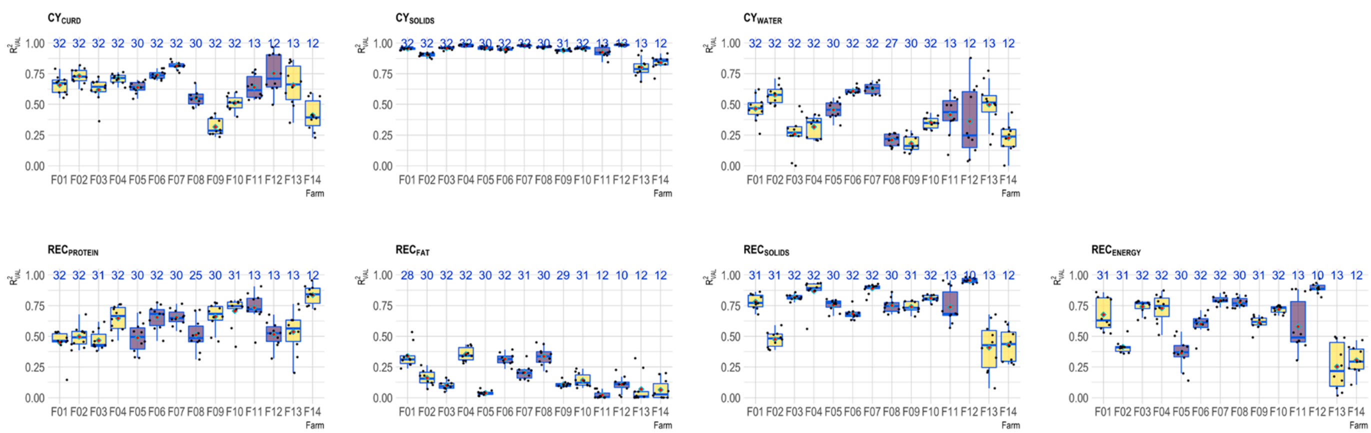


Fig. 3. Coefficient of determination of validation (R^2_{VAL}) results per farm (F01 to F14; purple boxes refer to extensive farms; yellow boxes refer to semi-extensive farms) of cheese-making traits obtained by 9-MilCA[1] using FTIR spectroscopy on individual goat milk samples in the SCV_{80} procedure[2]. Vertical lines within each boxplot represent the median, and red rhombus is the mean of the ten replicates per farm. Blue numbers on top refer to the number of goats in validation per farm. [1]Cheese yields (%CY; weight of fresh curd, curd solids, and curd water as percentage of weight of milk processed); milk nutrients recovery in the curd (%REC; weight of the curd component (protein, fat, total solids, energy) to the same component in milk, multiplied by 100). [2]Each farm was evaluated separately with 20 % of the farm included in the calibration set. The procedure was repeated ten times per farm (black dots). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

more by factors related to the individuals (i.e., ~ 80 % of the total variance was attributed to the animal) than those related to the farm (i.e., < 10 %).

Regarding $\%CY_{WATER}$, it has been previously evidenced that this is the most difficult trait to monitor during milk processing, being the least repeatable in the present study (0.93). This is in line with Cipolat-Gotet et al. (2016) that reported the lowest values of repeatability for $\%CY_{WATER}$ among cheese-making traits in bovine milk. We also found that SCV results might have been influenced by the day of cheese-making, since milk samples from each farm were processed separately. As aforementioned, $\%REC_{FAT}$ had the lowest prediction accuracies among all traits (Table 2), with average R^2_{VAL} among farms < 0.40, and a decrease of>50 % in SCV compared to the CV. Respect to $\%CY_{WATER}$, results among farms for $\%REC_{FAT}$ showed a low within-farm variability (Fig. 3). An explanation for prediction performances in $\%REC_{FAT}$ among farms could be given by the distribution in the size of the fat globules and the differences in single fatty acids, characteristics that are highly variable among farms with different feeding regimens (Lopez et al., 2008). For instance, differences in the recovery of short-chain SFA (lower recovery) and of C18:3n-6 (higher recovery) in the curd were observed by Cattani et al. (2014) assessing milk from cows fed with different levels of extruded flaxseed.

The inclusion of 20 % of the VAL farm in the CAL set (SCV_{80}) linked CAL and VAL sets, so that they were not completely independent (Fig. 2). On average, R^2_{VAL} results of the SCV_{80} were comparable to the SCV procedure, namely $0.62_{[0.23,0.97]}$, $0.94_{[0.68,0.99]}$, $0.40_{[0.00,0.88]}$ for %CY (curd, solids and water) and $0.60_{[0.14,0.96]}$, $0.17_{[0.00,0.53]}$, $0.72_{[0.08,0.98]}$, and $0.60_{[0.02,0.97]}$ for %REC (protein, fat solids and energy) traits, respectively. Roberts et al. (2017) observed an effect of overestimation of prediction accuracies using CV procedures in ecological data with dependence structures. On the contrary, we observed comparable average of R^2_{VAL} values moving from the SCV to the SCV_{80} for all the traits but with a different increase of the $R^2_{INTERVAL}$. Particularly, this result is not related to the prediction performances observed for each trait but could be partly due to the different within-farm variability among farms. Moreover, considerable variation was observed among farms for almost all the %CY and %REC traits, except for $\%CY_{SOLIDS}$. For this trait, the R^2_{VAL} was stable across farms (Fig. 3). although there were 2 farms (i.e., F13-14) with mean R^2_{VAL} < 0.85 over the 10 random replicates. Among cheese-making traits, $\%REC_{SOLIDS}$ showed higher within-farm variability compared to $\%CY_{SOLIDS}$ (Fig. 3). Interestingly, the ranking among farms was very similar between $\%CY_{SOLIDS}$ and $\%REC_{SOLIDS}$ that differed for the mean R^2_{VAL} and the extent of within-farm variability. In opposite, $\%CY_{WATER}$ and $\%REC_{FAT}$ had the worst R^2_{VAL} in the SCV and, again, different patterns among farms, with lower variability for $\%REC_{FAT}$. These results are consistent with the findings of Dadousis et al. (2021), who analyzed milk coagulation properties of the same dataset. More precisely, those authors reported large differences among farms for the gelation time and the asymptotic curd firmness and no relationships among traits. On the contrary, we observed that results of SCV_{80} for $\%CY_{CURD}$ were conditioned by $\%CY_{WATER}$ and results for $\%REC_{ENERGY}$ were affected by $\%REC_{SOLIDS}$. These connections do not depend so much on factors related to the farms, but rather on the technological meaning of these traits.

4. Implications for future development of portable IR instruments

Infrared spectroscopy (IR) has been routinely used to predict the chemical composition of milk in most herd recording programs, where benchtop instruments are employed in several laboratories involved in the official routine milk-recording systems. Quality requirements in the dairy industry are increasingly promoting the need of techniques enabling real-time monitoring of cheese-making processes and products, at the farm, dairy plant and population (for breeding purposes) levels. Therefore, portable and hand-held equipment represent the pioneering tools for milk quality control and real-time decisions. However, although some European countries (e.g., France, Spain, the Netherlands) are investing in the dairy goat sector, the cost for milk testing is still prohibitive for most of the dairy goat producers. To facilitate the implementation of IR calibration models in the field conditions, close collaborations among stakeholders of the dairy goat chain and companies producing IR instruments is recommended. Compared to the dairy cow sector, which is characterized by significant investments in facilities and technologies along the chain, that of goat is still considered marginal in the dairy industry. Hence, the results from this study on the prediction of important cheese-making traits for goat milk, derived from a benchtop instrument, guarantee the enhancement of the research and technology advancement within this topic and could pioneer the development of prediction models using portable IR Instruments.

5. Conclusions

In this study, we examined the feasibility of using milk FTIR spectroscopy to predict cheese-making traits in dairy goats and assessed the effect of farm on prediction accuracy. The consistent high prediction accuracy (on average > 0.9) in extended CV schemes and among farms for $\%CY_{SOLIDS}$, justifies its practical application. Although for the rest of traits prediction accuracies were lower respect to $\%CY_{SOLIDS}$, and varied among traits and farms, overall results were similar to or outperformed those previously reported for bovine milk. Moreover, our study demonstrated the importance of among-farm and within-farm variability in relation to predicting cheese-making traits via milk spectra obtained with FTIR spectroscopy. Our results highlighted the importance of considering specific procedures for calibration development to avoid misleading results and to produce realistic data applicable along the dairy chain.

CRediT authorship contribution statement

Giorgia Stocco: Conceptualization, Software, Validation, Formal analysis, Writing – original draft, Writing – review & editing. **Christos Dadousis:** Methodology, Software, Writing – review & editing, Formal analysis. **Michele Pazzola:** Investigation, Writing – review & editing, Supervision. **Giuseppe M. Vacca:** Conceptualization, Formal analysis, Funding acquisition. **Maria L. Dettori:** Formal analysis, Writing – review & editing. **Elena Mariani:** Software, Writing – review & editing. **Claudio Cipolat-Gotet:** Conceptualization, Methodology, Investigation, Writing – original draft, Writing – review & editing, Supervision.

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.

Data availability

Data will be made available on request.

Acknowledgments

This work was supported by the Regional Government of Sardinia (Progetto Strategico Sulcis; CUP J73C17000070007, Cagliari, Italy). The authors thank the farmers for giving access to their flocks; the APAs (Provincial Farmers Associations) of Cagliari and Nuoro (Italy), and the firms Società Agricola is Crabaxius (Fluminimaggiore, Italy), Azienda Agricola Murgia Antonello (Sant'Anna Arresi, Italy), Latteria Sociale Santadi (Santadi, Italy), Azienda Agricola F.lli Secci s.s. (Iglesias, Italy), and Agricola Allevatori Tallaroga, Soc. Coop. (Villamassargia, Italy) for their support in sample collection; and ARA Sardegna (Regional Farmers Association of Sardinia, Cagliari, Italy) for support in chemical milk analysis. The authors have not stated any conflicts of interest.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.foodchem.2022.134403.

References

Bittante, G., & Cecchinato, A. (2013). Genetic analysis of the Fourier-transform infrared spectra of bovine milk with emphasis on individual wavelengths related to specific chemical bonds. *Journal of Dairy Science, 96*, 5991–6006. https://doi.org/10.3168/jds.2013-6583

Bittante, G., Cipolat-Gotet, C., & Cecchinato, A. (2013). Genetic parameters of different measures of cheese-yield and milk nutrient recovery from an individual model cheese-manufacturing process. *Journal of Dairy Science, 96*, 7966–7979. https://doi.org/10.3168/jds.2012-6517

Bittante, G., & Cipolat-Gotet, C. (2018). Direct and indirect predictions of enteric methane daily production, yield, and intensity per unit of milk and cheese, from fatty acids and milk Fourier transform infrared spectra. *Journal of Dairy Science, 101*, 7219–7235. https://doi.org/10.3168/jds.2017-14289

Cattani, M., Mantovani, R., Schiavon, S., Bittante, G., & Bailoni, L. (2014). Recovery of n-3 polyunsaturated fatty acids and conjugated linoleic acids in ripened cheese obtained from milk of cows fed different levels of extruded flaxseed. *Journal of Dairy Science, 97*, 123–135. https://doi.org/10.3168/jds.2013-7213

Cellesi, M., Correddu, F., Manca, M. G., Serdino, J., Gaspa, G., Dimauro, C., & Macciotta, N. P. P. (2019). Prediction of Milk Coagulation Properties and Individual Cheese Yield in Sheep Using Partial Least Squares Regression. *Animals., 9*, 663. https://doi.org/10.3390/ani9090663

Chessa, S., Bulgari, O., Rizzi, R., Calamari, L., Biffani, S., & Caroli, A. M. (2014). Selection for milk coagulation properties predicted by Fourier transform infrared spectroscopy in the Italian Holstein-Friesian. *Journal of Dairy Science, 97*, 4512–4521. https://doi.org/10.3168/jds.2013-7798

Cipolat-Gotet, C., Cecchinato, A., Stocco, G., & Bittante, G. (2016). The 9-MilCA method as a rapid, partly automated protocol for simultaneously recording milk coagulation, curd firming, syneresis, cheese yield, and curd nutrients recovery or whey loss. *Journal of Dairy Science, 99*, 1065–1082. https://doi.org/10.3168/jds.2015-9734

Dadousis, C., Cipolat-Gotet, C., Stocco, G., Ferragina, A., Dettori, M. L., Pazzola, M., do Nascimento Rangel, A. H., & Vacca, G. M. (2021). Goat farm variability affects milk Fourier-transform infrared spectra used for predicting coagulation properties. Journal of Dairy Science, *104*, 3927-3935. 10.3168/jds.2020-19587.

de los Campos, G., & Perez Rodriguez, P. (2015). BGLR: Bayesian Generalized Linear Regression. R package version 1.0.4. Accessed July 15, 2021. http://CRAN.R-project.org/package=BGLR.

El Jabri, M., Sanchez, M.-P., Trossat, P., Laithier, C., Wolf, V., Grosperrin, P., … Delacroix-Buchet, A. (2019). Comparison of Bayesian and partial least squares regression methods for mid-infrared prediction of cheese-making properties in Montbéliarde cows. *Journal of Dairy Science, 102*, 6943–6958. https://doi.org/10.3168/jds.2019-16320

Ferragina, A., Cipolat-Gotet, C., Cecchinato, A., Pazzola, M., Dettori, M. L., Vacca, G. M., & Bittante, G. (2017). Prediction and repeatability of milk coagulation properties and curd-firming modeling parameters of ovine milk using Fourier-transform infrared spectroscopy and Bayesian models. *Journal of Dairy Science, 100*, 3526–3538. https://doi.org/10.3168/jds.2016-12226

Ferragina, A., de los Campos, G., Vazquez, A. I., Cecchinato, A., & Bittante, G. (2015). Bayesian regression models outperform partial least squares methods for predicting milk components and technological properties using infrared spectral data. *Journal of Dairy Science*, *98*, 8133-8151. 10.3168/jds.2014-9143.

ICAR (International Committee for Animal Recording). 2021. Guidelines: Section 12 - Milk Analysis. Accessed September 10, 2021. https://www.icar.org/index.php/icar-recording-guidelines/.

IDF, 2013. International Organization for Standardization and International Dairy Federation. Milk and liquid milk products. Determination of fat, protein, casein, lactose and pH content. International Standard ISO 9622 and IDF 141:2013. ISO, Geneva, Switzerland, and IDF, Brussels, Belgium (2013).

Kandel, P. B., Vanrobays, M.-L., Vanlierde, A., Dehareng, F., Froidmont, E., Gengler, N., & Soyeurt, H. (2017). Genetic parameters of mid-infrared methane predictions and their relationships with milk production traits in Holstein cattle. *Journal of Dairy Science, 100*, 5578–5591. https://doi.org/10.3168/jds.2016-11954

Kaylegian, K. E., Lynch, J. M., Fleming, J. R., & Barbano, D. M. (2009). Influence of fatty acid chain length and unsaturation on midinfrared milk analysis. *Journal of Dairy Science, 92*, 2485–2501. https://doi.org/10.3168/jds.2008-1910

Lopez, C., Briard-Bion, V., Menard, O., Rousseau, F., Pradel, P., & Besle, J.-M. (2008). Phospholipid, sphingolipid, and fatty acid compositions of the milk fat globule membrane are modified by diet. *Journal of Agricultural and Food Chemistry, 56*, 5226–5236. https://doi.org/10.1021/jf7036104

McParland, S., Lewis, E., Kennedy, E., Moore, S. G., McCarthy, B., O'Donovan, M., … Berry, D. P. (2014). Mid-infrared spectrometry of milk as a predictor of feed intake and efficiency in lactating dairy cows. *Journal of Dairy Science, 97*, 5863–5871. https://doi.org/10.3168/jds.2014-8214

Melilli, C., Lynch, J. M., Carpino, S., Barbano, D. M., Licitra, G., & Cappa, A. (2002). An empirical method for prediction of cheese yield. *Journal of Dairy Science, 85*, 2699–2704. https://doi.org/10.3168/jds.S0022-0302(02)74356-7

Mrode, R., Dzivenu, C. E., Marshall, K., Chagunda, M. G. G., Muasa, B. S., Ojango, J., & Okey, A. M. (2020). Phenomics and its potential impact on livestock development in low-income countries: Innovative applications of emerging related digital technology. *Animal Frontiers, 10*, 6–11. https://doi.org/10.1093/af/vfaa002

Nicolaou, N., Xu, Y., & Goodacre, R. (2010). Fourier transform infrared spectroscopy and multivariate analysis for the detection and quantification of different milk species. *Journal of Dairy Science, 93*, 5651–5660. https://doi.org/10.3168/jds.2010-3619

NRC (Nutrient Requirements of Dairy Cattle). (2001). Nutrient 7th rev. ed. Natl. Acad. Press, Washington, DC.

Othmane, M. H., Carriedo, J. A., de la Fuente Crespo, L. F., & San Primitivo, F. (2002). An individual laboratory cheese-making method for selection in dairy ewes. *Small Ruminant Research, 45*, 67–73. https://doi.org/10.1016/S0921-4488(02)00079-2

Paschino, P., Stocco, G., Dettori, M. L., Pazzola, M., Marongiu, M. L., Pilo, C. E., … Vacca, G. M. (2020). Characterization of milk composition, coagulation properties and cheese-making ability of goats reared in extensive farms. *Journal of Dairy Science, 103*, 5830–5843. https://doi.org/10.3168/jds.2019-17805

Pazzola, M., Stocco, G., Dettori, M. L., Bittante, G., & Vacca, G. M. (2019). Effect of goat milk composition on cheese-making traits and daily cheese productions. *Journal of Dairy Science, 102*, 3947–3955. https://doi.org/10.3168/jds.2018-15397

Picque, D., Lefier, D., Grappin, R., & Corrieu, G. (1993). Monitoring of fermentation by infrared spectrometry: Alcoholic and lactic fermentations. *Analytica Chimica Acta, 279*, 67–72.

Puledda, A., Gaspa, G., Manca, M. G., Serdino, J., Urgeghe, P. P., Dimauro, C., … Macciotta, N. P. P. (2017). Estimates of heritability and genetic correlations for milk coagulation properties and individual laboratory cheese yield in Sarda ewes. *Animal, 11*, 920–928. https://doi.org/10.1017/S1751731116002147

R Core Team (2013). R: A language and environment for statistical computing. Vienna, Austria: The R Foundation for Statistical Computing. Accessed September 10, 2021. http://www.R-project.org.

Roberts, D. R., Bahn, V., Ciuti, S., Boyce, M. S., Elith, J., Guillera-Arroita, G., … Dormann, C. F. (2017). Cross-validation strategies for data with temporal, spatial, hierarchical, or phylogenetic structure. *Ecography, 40*, 913–929. https://doi.org/10.1111/ecog.02881

Salleh, N. A., Selamat, J., Meng, G. Y., Abas, F., Jambari, N. N., & Khatib, A. (2019). Fourier transform infrared spectroscopy and multivariate analysis of milk from different goat breeds. *International Journal of Food Properties, 22*, 1673–1683. https://doi.org/10.1080/10942912.2019.1668803

Stocco, G., Dadousis, C., Vacca, G. M., Pazzola, M., Paschino, P., Dettori, M. L., … Cipolat-Gotet, C. (2021). Breed of goat affects the prediction accuracy of milk coagulation properties using Fourier-transform infrared spectroscopy. *Journal of Dairy Science, 104*, 3956–3969. https://doi.org/10.3168/jds.2020-19491

Stuart, B. H. (2004). *Infrared Spectroscopy: Fundamentals and Applications*. John Wiley & Sons.

Tiplady, K. M., Sherlock, R. G., Littlejohn, M. D., Pryce, J. E., Davis, S. R., Garrick, D. J., … Harris, B. L. (2019). Strategies for noise reduction and standardization of milk mid-infrared spectra from dairy cattle. *Journal of Dairy Science, 102*, 6357–6372. https://doi.org/10.3168/jds.2018-16144

Tiplady, K. M., Lopdell, T. J., Reynolds, E., Sherlock, R. G., Keehan, M., Johnson, T. J. J., … Littlejohn, M. D. (2021). Sequence-based genome-wide association study of individual milk mid-infrared wavenumbers in mixed-breed dairy cattle. *Genetics Selection Evolution, 53*, 62. https://doi.org/10.1186/s12711-021-00648-9

Vacca, G. M., Stocco, G., Dettori, M. L., Bittante, G., & Pazzola, M. (2020). Goat cheese yield and recovery of fat, protein, and total solids in curd are affected by milk coagulation properties. *Journal of Dairy Science, 103*, 1352–1365. https://doi.org/10.3168/jds.2019-16424

Vacca, G. M., Stocco, G., Dettori, M. L., Summer, A., Cipolat-Gotet, C., Bittante, G., & Pazzola, M. (2018). Cheese yield, cheese-making efficiency, and daily production of 6 breeds of goats. *Journal of Dairy Science, 101*, 7817–7832. https://doi.org/10.3168/jds.2018-14450

Valenti, B., Martin, B., Andueza, D., Leroux, C., Labonne, C., La-halle, F., … Ferlay, A. (2013). Infrared spectroscopic methods for the discrimination of cows' milk according to the feeding system, cow breed and altitude of the dairy farm. *International Dairy Journal, 32*, 26–32. https://doi.org/10.1016/j.idairyj.2013.02.014

Visentin, G., McDermott, A., McParland, S., Berry, D. P., Kenny, O. A., Brodkorb, A., … De Marchi, M. (2015). Prediction of bovine milk technological traits from mid-infrared spectroscopy analysis in dairy cows. *Journal of Dairy Science, 98*, 6620–6629. https://doi.org/10.3168/jds.2015-9323

Wang, Q., & Bovenhuis, H. (2019). Validation strategy can result in an overoptimistic view of the ability of milk infrared spectra to predict methane emission of dairy cattle. *Journal of Dairy Science, 102*, 6288–6295. https://doi.org/10.3168/jds.2018-15684

Wedholm, A., Larsen, L. B., Lindmark-Mansson, H., Karlsson, A. H., & Andren, A. (2006). Effect of protein composition on the cheesemaking properties of milk from individual dairy cows. *Journal of Dairy Science, 89*, 3296–3305. https://doi.org/10.3168/jds.S0022-0302(06)72366-9

Williams, P. (2007). Statistical terms for evaluation of accuracy and precision. Pages 5-1-5-17 in *Near Infrared Technology: Getting the Best Out of Light* (5th ed.). PDK Grain, Nanaimo, BC, and Winnipeg, Manitoba, Canada.