J. Dairy Sci. TBC
https://doi.org/10.3168/jds.2023-24005

The ability of a handheld near-infrared spectrometer for a rapid quality assessment of bovine colostrum including the Ig G concentration

Arianna Goi,[1] Angela Costa,[2]* and Massimo De Marchi[1]
[1]Department of Agronomy, Food, Natural resources, Animals and Environment, University of Padova, Viale dell'Università 16, 35020 Legnaro (PD), Italy
[2]Department of Veterinary Medical Sciences, University of Bologna, via Tolara di Sopra 50, 40064 Ozzano dell'Emilia (BO), Italy

ABSTRACT

Portable infrared-based instruments have made significant contributions in different research fields. Within the dairy supply chain, for example, most of portable devices are based on near-infrared spectroscopy (NIRS) and are nowadays an important support for farmers and operators of the dairy sector, allowing fast decision-making, particularly for feed and milk quality evaluation and animal health and welfare monitoring. The affordability, portability, and ease of use of these innovative devices have been pivotal factors for the implementation in dairy farms. In fact, pocket-sized devices enable non-expert users to perform quick, low cost and non-destructive analysis on various samples without complex preparation. As bovine colostrum (BC) quality is mostly given by the Ig G (IgG) level, evaluating the ability of portable NIRS tools to measure antibodies concentration is advisable. In this study we used the wireless device SCiO manufactured by Consumer Physics Inc. (Tel Aviv, Israel) to collect BC spectra and then attempt to predict IgG concentration and gross and fine composition in individual samples collected as soon as possible after calving (<6 h) in primiparous and pluriparous Holstein cows farmed in 9 Italian farms. Chemometric analyses revealed that SCiO has promising predictive performance for colostral IgG concentration, total Ig concentration, fat, and AA ($R^2_{CV} \geq 0.75$). Excellent accuracy was observed for dry matter, protein, and S prediction in cross-validation and good prediction ability in external validation ($R^2_{CV} \geq 0.93$; $R^2_{V} \geq 0.82$). Nonetheless, SCiO's ability to discriminate between good- and low-quality samples was satisfactory. The affordable cost, the accurate predictions, and the user-friendly design coupled with the increased interest in colostrum quality within the dairy sector may boost the collection of extensive BC data for management and genetic purposes in the near future.
Key words: colostrum, dairy cattle, portable instrument, spectroscopy, passive transfer of immunity

INTRODUCTION

In the dairy sector, infrared spectroscopy-based technologies are acknowledged to be moderately to highly accurate, have been widely accepted by stakeholders, and are implemented for various purposes. As cheap, sometimes portable, and easy to use, infrared-based tools have boosted the improvement of knowledge and transition toward better management practices, including animal health and welfare monitoring. In the case of milk and dairy products, the spectral hotspots mostly belong to the near- (800–2,500 nm) and mid-infrared (2,500–25,000 nm) regions. If on one hand mid-infrared spectroscopy is used worldwide for the collection of milk composition traits to be used as phenotypes for milk payment and genetic evaluation, near-infrared spectroscopy (**NIRS**) is the most popular technology for rapid quality assessment of solid and semi-solid material like feed and foodstuff (curd, cheese, yogurt, etc.). The repeatability, reproducibility, and overall accuracy of benchtop instruments is so good that NIRS has been recognized as a gold standard for gross composition (ISO 21543:2020) of milk and derived products for official use.

In recent years, portable NIRS instruments have been promoted under the umbrella of precision livestock farming, paving the way for rapid and customized decision-making in dairy farms (Evangelista et al., 2021; Pu et al., 2021). In fact, benchtop instruments as well as the pocket-size devices can ensure a rapid and non-destructive analysis of a variety of matrices, which can be performed by non-expert users after brief training. Furthermore, preparation of samples is minimum and easy. In terms of accuracy, portable devices are generally less performing than benchtop ones. This is due to the usually worse wavelength reproducibility, lower resolution, reduced spectral range (Sun et al., 2020;

Received July 24, 2023.
Accepted January 24, 2024.
*Corresponding author: Dr Angela Costa, Department of Veterinary Medical Sciences, University of Bologna, via Tolara di Sopra 50, 40064 Ozzano dell'Emilia (BO), Italy, angela.costa2@unibo.it

Mishra et al., 2021), and to the quality of pre-existing models already installed. Prediction accuracy of NIRS instruments is, in fact, related to the goodness of the built equation(s) which has to be robust and developed in such a way as to avoid overfitting. The majority of micro-spectrometers – e.g., SCiO (Consumer Physics Inc., Tel Aviv, Israel), NIRONE 2.2 (Spectral En109 gines, Finland), or F750 (Felix Instrument, Camas, USA) – are designed to allow technicians to develop and install customized prediction models (Ryckewaert et al., 2022). Moreover, they are specifically designed to be suitable for operation by non-expert users, such as farmers, through pre-developed software/APP that ensures ease of use (Beć et al., 2020). At the same time, NIRS predictions are directly affected by the precision of the reference method used (Sørensen, 2002; Blanco and Peguero, 2010) and by the intrinsic characteristics of the samples undergoing analysis. In fact, the most reliable outcomes are obtained under standard conditions, i.e., in the presence of appropriate sample collection, manipulation, and scanning following the manufacturer's instructions.

Given its importance for neonatal calves and its recent industrial applications, bovine colostrum (**BC**) nowadays represents one of the most interesting semi-solid matrices to be analyzed with low-cost portable tools within the whole dairy supply chain, not only at farm level (Costa et al., 2023). It has been demonstrated that BC composition is highly variable in the first hours after calving; in particular, this is the case for the narrow-sense quality of BC, mostly given by the concentration of Ig, particularly of the isotype G (**IgG**). Although for different reasons, from both producers' and farmers' standpoint, IgG is the most important criterion to evaluate BC quality. In fact, high concentration of IgG in BC coupled with good feeding and management practices reduces the risk of passive transfer failure in neonatal calves. At the same time, commercial manufacturers of food or pharmaceutical items containing BC are willing to pay "more" if the concentration of antibodies in the supplied volume is good (Costa et al., 2023). Conventionally, veterinarians and farmers consider BC with IgG <50 g/L as of insufficient quality for calves feeding, especially at first meal. This threshold has international validity (Godden et al., 2019). To optimize calves' survival in a precision feeding view, the possibility to measure the IgG level of both pooled or individual BC with portable NIRS tools becomes thereby interesting in this scenario.

The aim of the present study was to evaluate the predictive ability of a wireless hand-held near-infrared spectrometer (SCiO, Consumer Physics Inc., Tel Aviv, Israel), for at-farm evaluation of BC IgG concentration, gross and fine composition through home-made equations. The possibility to record sufficiently accurate IgG data in the field would, in fact, improve the knowledge about the farm BC quality, putting the basis for the definition of strategic precision feeding in non-suckling calves.

MATERIALS AND METHODS

Sampling

Ethical approval was not required for the present study as per institutional guidelines/local legislation, since only farmers interacted with the cows. The animals' owners involved in the study signed a written informed consent, joined the experiment on a voluntary basis, and were associated with the Veneto Region Breeders Association (**ARAV**, Vicenza, Italy). Individual samples of 709 purebred Holstein cows, 215 primiparous and 494 pluriparous, that calved between spring 2019 and spring 2020 were collected from 9 commercial farms located in North-East Italy as described by Costa et al. (2022) and Goi at al. (2023a). Overall, the selected farms were characterized by an intensive farming system, free stall barn, total mixed ration administration, twice-a-day milking, and no access to pasture. The experimental design covered the variability of calving season and parity order, which ranged from 1 to 8 and averaged 2.47 ± 1.42. In line with the experimental protocol, calves were separated from dams immediately after birth, suckling was absent, and only the first colostrum (120 mL) was collected from each cow between 0 and 6 h after calving. The tubes used were sterile, made of polypropylene, and free of preservative (SMIPA srl, Vicenza, Italy); once filled, they were stored at −20°C (Costa et al., 2021a). Vaccination before calving against Rotavirus, Coronavirus, and *E. coli* was not performed in the donor cows to avoid presence of hyperimmune colostrum (Dunn et al., 2017; Costa et al., 2023).

Reference Analyses. The procedure carried out to perform the reference analyses is the same as described by Goi et al. (2023a, 2023b) following the workflow illustrated in Figure 1. Briefly, protein was measured by using the Kjeldahl method 991.20 (AOAC, 2000), fat content was determined according to Verbands Deutscher Landwirdschaftlicher Untersuchungs und Forschungsanstalten (**VDLUFA**) VI C15.2.1 method (VDLUFA, 2013), while lactose was quantified through high-performance liquid chromatography (Aminex HPX 87H column, 300 mm × 7.8 mm; Bio-Rad). Lactose concentration was determined through a chromatography software (ChromNAV v. 2.0, Jasco).

The concentration of Ig (isotype G, A, and M) was assessed using the bovine-specific radial-immunodiffu-

sion (**RID**) assay purchased from Triple J Farms (Bellingham, WA, US), whose repeatability has been tested by intra- and inter-assay CV, as described in detail by Costa et al. (2021b) and Goi et al. (2023a). The total Ig concentration (**IgTot**) was calculated as the sum of all isotypes exclusively for the samples with the 3 concentrations known.

Following the procedure already described by Goi et al. (2023b), for mineral quantification, a 2 mL aliquot was mineralized and then analyzed using ICP-OES SPECTRO ARCOS (SPECTRO Analytical Instruments GmbH, Kleve, Germany), whereas for AA quantification, a 15 mL aliquot of each sample was lyophilized, underwent acid hydrolysis and pre-column derivatization, and then was separated by a reversed-phase instrument of high-pressure liquid chromatography and analyzed by UV detection.

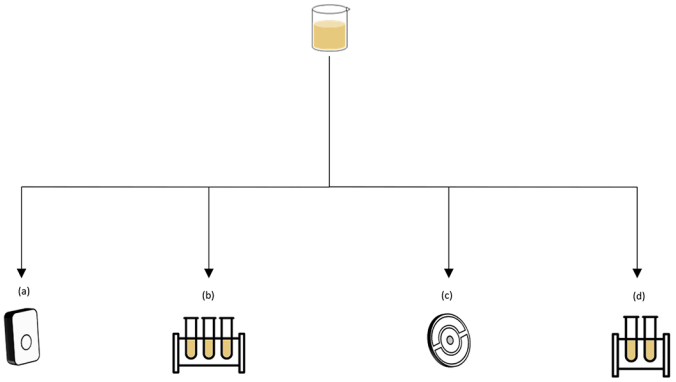

Figure 1. Workflow adopted according to the colostrum samples destination: (a) spectra collection through SCiO, (b) gross composition analyses with gold standards, (c) determination of Ig isotypes concentrations via radial-immunodiffusion assay, and (d) quantification of mineral and AA content.

Development of NIRS Models

Spectra of BC were recorded through SCiO (Consumer Physics Inc., Tel Aviv, Israel) which works in reflectance mode in the wavelength region between 740 and 1070 nm, at intervals of 1 nm. For this purpose, for each sample 50 mL of thawed BC was put in a sterile tube and left at room temperature for 1 h to standardize scanning conditions. Subsequently, before the scan, the tube was inverted to homogenize the sample. SCiO, equipped with a manufacturer-provided adapter featuring a ceramic bottom to scatter back the light emitted from the source toward the detector while passing through the matrix, was inserted directly into the test tube to record the spectra in transflectance mode. The instrument was also cleaned with sterile water and dried with a disposable towel between each sample.

For each sample, 3 spectra were stored and then the average was calculated. Spectral data points were converted from transflectance (Transfl) to absorbance (Abs) using the formula: Abs = $\log_{10}(1/\text{Transfl})$ and then used for the calibration once paired with the reference data. Reference outliers (values exceeding ± 3 SD from the mean) and spectral outliers (Mahalanobis distance >3) where discarded before developing calibration models.

For all the traits, chemometric analyses were performed using WinISI 4.10 software (Infrasoft International, Port Matilda, PA, USA) through a modified partial least squares (**mPLS**) regression algorithm. Preliminarily, different scatter corrections were tested on spectral data: none, detrend, standard normal variate, standard normal variate and detrend, and multiplicative scatter correction. Each of the mentioned pretreatment was tested in combination with mathematical treatments: 0,0,1,1; 1,4,4,1; 1,5,5,1; 1,8,8,1; 2,5,5,1, where the first digit is the derivative, the second digit is the gap over which the derivative was calculated, the third digit is the gap for the first smoothing, and the fourth is the gap for the second smoothing. Three steps of outliers' elimination were performed after each mPLS round (n = 3), at the end of which the samples whose predicted value differed more than ± 3 SE_{CV} (T-statistic >3) from the reference value were excluded.

The entire data set was first divided for each trait to create the training set, selecting randomly 75% of data, while the remaining 25% represented the external validation – or testing – set. The mean and SD of the 2 sets were ensured to be similar. The prediction equations were developed on the training set and internally tested performing a 5-fold cross-validation. To avoid overfitting, the number of latent variables (**LV**) which minimized the root-mean-square error of cross-validation were included in the model. In terms of predictive performance, the model with the lower standard error of cross-validation ($\mathbf{SE_{CV}}$) and the greater coefficient of determination of cross-validation ($\mathbf{R^2_{CV}}$) was elected as the best and underwent external validation. After that, for each trait the final model was applied to the external samples (testing set) where the reference values were masked. Performance in external validation was evaluated based on the greater coefficient of determination of external validation ($\mathbf{R^2_V}$) and the greater residual predictive deviation (**RPD**). Residuals normality was inspected and the TTEST procedure of SAS v. 9.4 (SAS Institute, NC, USA) was adopted to test that the bias did not statistically differ from zero.

A discriminant analysis was used on the entire set net of outliers to evaluate the classification ability of SCiO based on spectral wavelengths of BC. For this purpose, the PROC STEPDISC available in SAS v.

9.4 (SAS Institute, Cary, NC, USA) was used for a preliminary backward elimination of spectral regions. This step was followed by the PROC DISCRIM where 'low quality' and 'good quality' samples were identified using 3 IgG thresholds: 50, 60, and 70 g/L. The model performance included the specificity, sensitivity, the overall percentage of samples correctly classified, and the Matthews correlation coefficient (**MCC**) which was calculated based on the number of true positives (**TP**), false positives (**FP**), true negatives (**TN**) and false negatives (**FN**) as follows:

$$MCC = \frac{TP \times TN - FP \times FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}}.$$

Diagnostic Accuracy

The Receiver Operating Characteristic (ROC) curve was used to evaluate the diagnostic accuracy of the predicted IgG for the external validation set by using PROC LOGISTIC (SAS v. 9.4, SAS Institute, Cary, NC, USA). The same thresholds used for the discriminant analysis were adopted and the area under the curve (AUC; Šimundić, 2009) was finally used to evaluate the classification ability of the infrared-predicted IgG.

RESULTS AND DISCUSSION

In the present study, the predictive ability of SCiO for IgG and BC composition traits was tested using samples (n = 709) collected in 9 farms. The BC collection was done by the farm staff, preliminarily trained, using the same protocol and within 6 h from calving.

As the reference data derived from various analyses, i.e., different kits/devices/procedures, the final number of records available slightly differ across traits. Table 1 shows the number of samples with matching reference value and spectrum, net of outliers. In the case of RID, for example, 3 kits were available – one for each isotype. The final number of records for IgG, Ig of isotype A (**IgA**) and M (**IgM**), and IgTot (Table 1) differed; samples may be excluded due to not readable and non-circular RID rings, final calculated concentration out of the kit detection range, and missing/lost aliquot (Costa et al., 2021b).

Descriptive statistics indicates that IgG was the predominant fraction and was highly variable, ranging between 0.68 and 198.90 g/L. Nevertheless, this fraction was less variable compared with the other 2 isotypes. Overall, 75 samples were considered as of insufficient quality, having IgG <50 g/L, thus the vast majority presented a concentration above the conventional cut-off (Godden et al., 2019). Regarding gross composition, descriptive statistics are in line with findings of Gopal and Gill (2000) and Godden (2008). The highest CV was that of fat (67%) and the lowest CV (<19%) was obtained for ash and dry matter. The average fat content (4.64%; Table 1) is in agreement with Elfstrand et al. (2002; pooled samples from Swedish Friesian cows) but slightly lower than the average content reported by Kehoe et al. (2007; 6.70%) on individual BC samples collected within 4 h from calving in 55 cows. As reviewed by Costa et al. (2023), when comparing BC of different studies, it is important to highlight that dissimilarities may be due to the collection time interval after birth and the gold standard used for the analysis.

Distribution of AA and minerals values for each parameter was normal except for Fe (Table 1), which was indeed logarithmically transformed to obtain a normal distribution of the data points before performing the chemometric analysis. The most and least abundant AA were Leu (294.95 ± 121.51 mg/100g as is) and Met (48.23 ± 20.91 mg/100g as is), respectively. The ranking of AA in terms of concentration was the same as the one reported by Puppel et al. (2019) for BC, except for Arg whose concentration in the cited study was greater than Met. Small differences in terms of variability were noticed among the AA analyzed, as their CV ranged from 39.89% (Ile) to 45.44% (Thr). As regards the minerals, Ca and P were the most abundant with a concentration of around 2 g/kg as is of BC, followed by S and Zn whose concentration was around 1.4 g/kg as is (Table 1). Minerals present in low quantity were Na and Mg, followed by the 2 minor minerals (Zn and Fe). In general, the mineral content of BC in this study resembled the values reported by of Playford and Weiser (2021) about Ca, P, K, Na, Mg, and Zn. In contrast, Kehoe et al. (2007) – using BC of 55 cows – found greater average mineral concentrations compared with this study, i.e., the average of Ca, P, S, K, Na, Mg, Zn, and Fe was 4716.10, 4452.10, 2595.67, 2845.89, 1058.93, 733.24, 38.10, and 5.33 mg/kg as is.

Within the present study, CV of major minerals was generally lower than that of AA, moving from 14.87% (K) to 27.42 (Mg). On the contrary, minor minerals like Zn an Fe varied widely (CV of 36.51 and 46.45%, respectively). As indicated for gross composition, it is often difficult to fairly compare BC components determined in different studies. The concentration of fine composition traits like minerals and AA is known to be strongly affected by the sampling protocol used, feeding and husbandry system, and parity of the donor cow (Costa et al., 2021b).

Table 1. Descriptive statistics of bovine colostrum Ig[1] fractions, composition traits, AA, and minerals concentration measured with the reference method after outliers' elimination

Trait	n	Mean	SD	Min	Max	CV
Major compounds						
IgG, g/L	647	91.97	35.37	0.68	198.90	38.45
IgA, g/L	555	4.65	2.73	0.13	13.95	58.65
IgM, g/L	632	5.08	2.42	0.18	11.89	47.65
IgTot, g/L	554	102.88	36.00	17.96	196.86	34.99
Dry matter, %	685	24.04	4.52	10.30	36.61	18.82
Protein, %	688	14.49	3.73	4.26	25.22	25.72
Fat, %	679	4.64	3.10	0.12	14.67	66.79
Ash, %	683	1.14	0.18	0.63	1.68	15.58
Lactose, mg/100mg	701	2.37	0.53	0.74	4.06	22.34
AA, mg/100g as is						
Leu	684	294.95	121.51	20.38	670.74	41.20
Lys	681	281.45	116.26	20.42	646.55	41.31
Thr	683	225.94	102.66	12.26	546.76	45.44
Val	682	189.07	82.32	12.63	429.99	43.54
Phe	682	139.32	55.83	10.04	312.12	40.07
Arg	681	129.14	56.87	6.71	292.56	44.04
Ile	681	104.34	41.62	9.14	232.46	39.89
His	684	96.88	40.23	4.45	223.24	41.53
Trp	681	69.00	31.08	4.14	165.40	45.04
Met	682	48.23	20.91	5.10	111.43	43.35
Minerals, mg/kg as is						
Ca	683	2188.94	520.64	631.48	3694.25	23.79
P	684	1957.27	398.75	835.12	3113.15	20.37
S	686	1445.68	380.05	403.91	2533.64	26.29
K	684	1420.99	211.32	729.96	2068.66	14.87
Na	678	557.51	144.29	250.39	1082.69	25.88
Mg	681	339.08	92.96	107.13	637.18	27.42
Zn	681	20.28	7.41	2.86	42.23	36.51
Fe	672	1.37	0.64	0.32	5.09	46.45
Fe[2]	672	0.10	0.17	−0.50	0.71	172.17

[1]isotypes G (IgG), A (IgA), and M (IgM) and their sum (IgTot).

[2]log-transformed.

SCiO for Ig and Gross Composition

The advantages and applications of a rapid and inexpensive assessment of BC composition through infrared spectroscopy using benchtop instruments have been already discussed in literature (Navrátilová et al., 2006; Rivero et al., 2012; Franzoi et al., 2022; Goi et al., 2023a; Goi et al. 2023b). However, only few studies have investigated the application of portable devices for analysis of mammary gland secretions, either BC or milk. While portable devices have been used to detect adulterants in milk and to assess milk fat and fatty acids content (Santos et al., 2013; Amr et al., 2018; Llano Suárez et al., 2018), none has demonstrated doable and useful applications on BC so far.

Portable spectrometers can be used on-line and are time-saving when it comes to visualize and interpret outputs of the analysis. Obtaining real-time information on mammary gland secretions composition allows the farmer to evaluate the quality of the freshly collected BC or milk and immediately determine the most appropriate destination. In the case of BC, for example, banking is a popular management strategy especially in well managed herds. Having the possibility to determine the narrow-sense quality of BC to be stored is pivotal for calves' health and precision feeding. Potentially, infrared analysis can be performed quickly on the BC produced at first and subsequent milkings, e.g., transition milk.

The average raw absorbance spectra (740 – 1,070 nm) of BC is depicted in Figure 2 with its SD. The pattern presents a weak peak around 840 nm and a broad peak around 980 nm. The former is due to a combination of C-H vibrations and can be ascribed to any of the main milk components, whereas the latter arises from symmetric and asymmetric vibration of water (Šašić and Ozaki, 2001). As indicated by the dashed lines, a slightly wider variation was observed in correspondence of the water absorption band, likely due to the difference in solids content, especially lipids. As explained above, the BC fat content was much more variable than other constituents and can cause a shift in the spectrum (Rivero et al., 2012).

Table 2 and 3 report the predictive performances of the developed equations in cross- and external validation respectively, for the Ig fractions, gross com-

position, AA, and minerals along with the number of samples used in the final models. Overall, considering the Ig isotypes and the gross composition, the outliers eliminated have always been ≤12.1%, with the exception of fat, which suffered a slightly higher elimination of samples (14.7%). Outliers can be either in spectral data, chemical (reference) values, or both (Wang et al., 2018). In the case of BC, the number of outliers detected could be attributed to the viscosity of the matrix, which likely influenced the reflection of light on the ceramic surface of the adapter used in scanning the samples with the instrument (Williams, 2007). In the case of cross-validation of IgG (Table 2), for example, 34 of the 38 discarded samples had an outlier spectrum. Performing cross-validation on the entire data set, the number of LV oscillated between 5 and 10 and the mostly used scatter correction was detrend along with first derivative. On the other hand, the range of LV used for the external validation was almost the same as in the cross-validation being between 4 and 10, while the accuracy is slightly changed as expected (Table 3). In this case the standard normal variate alone or with detrend were the most frequently used corrections, with first or second derivative. In this study, SCiO demonstrated its ability to predict BC composition. In particular, according to the classification of R^2 and RPD made by Williams (2003; 2014), an approximate and sufficient ability to quantify IgG (R^2_{CV} = 0.78; RPD = 2.1) was observed in cross-validation (Table 2). The same can be said for IgTot (Table 2). More precisely, the formal interpretation of the RPD suggests that the models have the potential for qualitative evaluation or rough screening solely (Williams, 2003, 2014), limiting therefore the potential of SCiO for the IgG concentration assessment of such an important mammary gland secretion. Thus, considering the matrix's relevance in the farm for a good calves management and having in mind its complexity (e.g., viscosity) per se, achieving that level of accuracy in practice is deemed sufficient also for the compounds quantification (Williams, 2003, 2014). Moreover, attention should be given to the fact that pocket-sized instruments are designed to accept a relatively limited overall performance compared with benchtop ones, but with a benefit in terms of cost-effectiveness. Therefore, the accuracy of models obtained with spectral data from portable instruments may often not coincide and be inferior to that of laboratory instruments, but this is a necessary compromise to tailor the instruments to their specific field of application (Beć et al., 2022), in this particular case for use by private practitioner veterinarians or farmers.

Likely due to the low concentrations compared with IgG and IgTot, both IgA and IgM did not achieve a satisfactory prediction accuracy (R^2_{CV} < 0.66). The

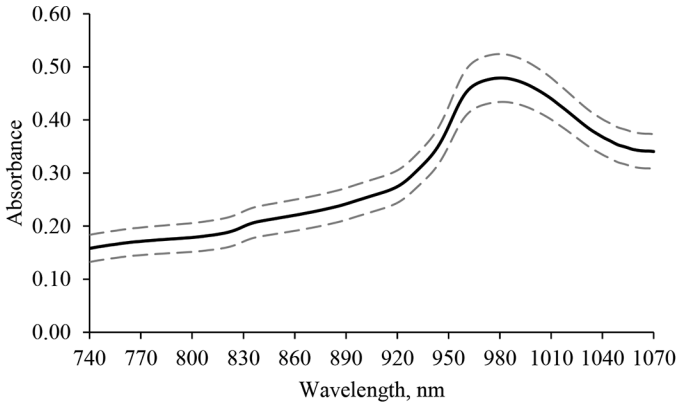

Figure 2. Average raw spectrum (n = 709, solid line) obtained using SCiO spectrometer. Dashed lines indicate the phenotypic variability observed (±1 standard deviation from the mean).

result for IgG is almost the same as that obtained by Elsohaby et al. (2018) with laboratory mid-infrared spectroscopy analysis on 60 cows within 1 h from calving, but lower than the accuracy reported by Rivero et al. (2012) scanning colostrum samples with the NIR Systems 6500 monochromator, a benchtop instrument. The performance related to the prediction of Ig remained unchanged when validating the models on the validation subset, with sufficient accuracy for an approximate quantification of the IgG (R^2_V = 0.80) and IgTot content (R^2_V = 0.70), while not satisfactory for the other 2 fractions (Table 3). This indicates that the developed models are able to be applied to samples with unknown values without noticing a change in precision. Also Franzoi et al. (2022), predicting IgG content using the DS2500 near-infrared benchtop spectrometer (400–2500 nm; FOSS, Hillerød, Denmark) showed no significant changes in prediction accuracy between cross- and external validation. Dry matter and protein content achieved excellent prediction accuracy in cross-validation, with $R^2_{CV} \geq 0.95$ and RPD ≥4.4, with this promising performance in agreement with the correlation coefficients reported by Navrátilová et al. (2006) for BC (Table 2). In that study, a benchtop NIRS instrument was used to evaluate its predictive ability scanning 90 colostrum samples collected from 18 cows over a wide time interval. A slight decrease of the accuracy was detected when validating externally the performances of the models ($R^2_V \geq 0.89$ and RPD ≥3.1), nevertheless indicating the adequacy of the predictive model to perform a quality control with a punctual determination of the traits (Table 3). Unfortunately, Navrátilová et al. (2006) did not perform the external validation to compare the data. Although the model developed for fat presented a lower accuracy compared with the other traits and compared

with Navrátilová et al. (2006), still the R^2_{CV} (0.86) and RPD (2.7) guarantee a satisfactory prediction. Applying an external validation, fat experiences a significant reduction in the R^2_V and RPD values (0.54 and 1.3, respectively), indicating that the model cannot provide a robust prediction (Williams, 2003; 2014). The scarce prediction performance can be attributed to the high variability of the reference data; the high content of solids in BC and the dilution may have affected the spectra. The rather low accuracy of lactose prediction indicates that only a discrimination between low and high concentration could be made (R^2_{CV} = 0.65; R^2_V = 0.61), whereas ash content did not achieve sufficient accuracy in both cross- (R^2_{CV} = 0.27) and external validation (R^2_V = 0.19); despite this, implementation of SCiO in the field is not or only marginally affected. In fact, still the most important parameter for the narrow-sense BC quality remains the IgG. This is true for both farmers and manufacturers interested in using BC as ingredient for industrial purpose (Costa et al., 2023). However, apart from the IgG, assessment of the gross composition would allow the real-time adjustment of the BC administered to calves, especially under a precision feeding view.

Prediction of Fine Composition Traits

To the authors′ knowledge no studies have attempted to predict essential AA and minerals content of BC using portable NIRS devices (Costa et al., 2023). However, with fine composition we refer to traits important for the broad-sense quality of BC, including substances fundamental for the neonate growth and health. According to the results, it is possible to predict AA and minerals content; performance obtained in cross-validation on the total data set and in external validation on the data set divided into training and testing sets are summarized in Table 2 and 3, respectively. The outliers detected during the calibration process were below 13% for all the traits, excepting K and Na. The number

Table 2. Fitting statistics[1] of modified partial least square regression analysis in 5-fold cross-validation for bovine colostrum Ig[2], gross composition, AA, and minerals (% on kg as is) on the entire set

Trait	sc−mt[4]	Out	LV	SE_C	R^2_C	SE_{CV}	R^2_{CV}	RPD
Major compounds								
IgG, g/L	D−2,5,5,1	5.9	6	15.74	0.80	16.50	0.78	2.12
IgA, g/L	D−1,4,4,1	12.1	6	1.77	0.48	1.84	0.44	1.33
IgM, g/L	D−1,8,8,1	7.6	5	1.80	0.43	1.82	0.41	1.30
IgTot, g/L	None−1,5,5,1	9.9	7	17.30	0.76	17.64	0.75	2.02
Dry matter, %	D−2,5,5,1	9.8	7	0.92	0.95	0.97	0.95	4.41
Protein, %	None−2,5,5,1	7.3	10	0.72	0.96	0.78	0.96	4.72
Fat, %	SNV−1,4,4,1	14.7	5	1.06	0.87	1.08	0.86	2.68
Ash, %	SNVD−0,0,1,1	10.7	7	0.14	0.30	0.15	0.27	1.17
Lactose, mg/100mg	D−1,8,8,1	11.4	9	0.27	0.68	0.29	0.65	1.69
AA, mg/100g as is								
Leu	SNVD−1,5,5,1	11.0	7	44.09	0.85	45.63	0.84	2.59
Lys	D−2,5,5,1	7.2	8	45.51	0.83	47.35	0.82	2.43
Thr	SNV−1,4,4,1	11.0	7	38.77	0.84	39.71	0.83	2.49
Val	MSC−1,4,4,1	12.5	7	31.09	0.84	31.69	0.83	2.46
Phe	SNV−1,5,5,1	11.6	8	19.63	0.86	20.07	0.86	2.69
Arg	MSC−1,4,4,1	11.6	8	20.95	0.85	21.78	0.84	2.57
Ile	MSC−1,5,5,1	11.2	8	17.05	0.81	17.55	0.80	2.32
His	MSC−1,4,4,1	11.8	7	15.82	0.82	16.13	0.82	2.39
Trp	D−0,0,1,1	10.1	11	12.50	0.82	12.98	0.81	2.38
Met	MSC−1,5,5,1	10.6	9	9.42	0.77	9.81	0.75	2.10
Minerals, mg/kg as is								
Ca	MSC−1,4,4,1	9.22	6	403.28	0.37	412.68	0.34	1.24
P	SNV−1,5,5,1	9.94	5	316.79	0.34	320.57	0.32	1.21
S	D−2,5,5,1	8.75	7	92.80	0.94	97.41	0.93	3.80
K	MSC−0,0,1,1	20.03	6	189.58	0.10	192.23	0.07	1.04
Na	SNV−1,8,8,1	17.11	6	118.98	0.12	121.11	0.09	1.05
Mg	MSC−1,4,4,1	10.28	6	65.02	0.46	66.11	0.44	1.34
Zn	SNV−1,5,5,1	9.84	6	5.49	0.41	5.61	0.38	1.27
Fe[3]	None−2,5,5,1	10.57	9	0.10	0.50	0.11	0.43	1.33

[1]sc−mt = scatter correction − mathematical treatment; Out = percentage of outliers; LV = latent variables; SE_C = standard error of calibration; R^2_C = coefficient of determination of calibration; SE_{CV} = standard error of cross-validation; R^2_{CV} = coefficient of determination of cross-validation; RPD = residual predictive deviation.

[2]isotypes G (IgG), A (IgA), and M (IgM) and their sum (IgTot).

[3]log-transformed.

[4]Detrend (d), Multiplicative scatter correction (MSC), No scatter correction (None), Standard normal variate (SNV), Standard normal variate+Detrend (SNVD).

Table 3. Fitting statistics[1] of modified partial least square regression analysis in external validation for bovine colostrum Ig[2], gross composition, AA, and minerals

Trait	Sc−mt[4]	n_{ext}	LV	SE_V	R^2_V	RPD
Major compounds						
IgG, g/L	D−1,4,4,1	150	10	16.05	0.80	2.22
IgA, g/L	SNV−1,5,5,1	134	7	1.94	0.46	1.41
IgM, g/L	SNV−1,8,8,1	149	5	1.94	0.37	1.25
IgTot, g/L	None−2,5,5,1	137	4	19.98	0.70	1.82
Dry matter, %	D−2,5,5,1	169	6	1.51	0.89	3.07
Protein, %	None−1,5,5,1	163	10	1.10	0.92	3.39
Fat, %	SNVD−2,5,5,1	170	4	2.43	0.54	1.28
Ash, %	MSC−2,5,5,1	171	5	0.16	0.19	1.10
Lactose, mg/100mg	D−0,0,1,1	167	10	0.33	0.61	1.65
AA, mg/100g as is						
Leu	SNV−1,4,4,1	168	7	58.82	0.77	2.06
Lys	SNVD−0,0,1,1	162	10	62.15	0.72	1.90
Thr	SNV−1,4,4,1	164	7	43.94	0.82	2.34
Val	SNVD−1,8,8,1	171	7	47.15	0.69	1.77
Phe	SNV−1,4,4,1	165	7	24.05	0.82	2.34
Arg	SNV−2,5,5,1	163	5	27.51	0.76	2.10
Ile	MSC−1,8,8,1	161	9	21.49	0.73	1.97
His	D−2,5,5,1	165	5	20.16	0.73	1.99
Trp	D−2,5,5,1	168	4	15.61	0.75	2.03
Met	SNV−1,4,4,1	164	8	11.01	0.72	1.92
Minerals, mg/kg as is						
Ca	None−1,5,5,1	162	6	444.37	0.26	1.18
P	SNVD−0,0,1,1	162	7	354.18	0.25	1.13
S	D−1,4,4,1	163	7	166.10	0.82	2.31
K	MSC−2,5,5,1	167	2	214.68	0.03	0.99
Na	MSC−0,0,1,1	170	7	145.92	0.04	1.00
Mg	MSC−2,5,5,1	171	4	71.02	0.44	1.33
Zn	SNVD−1,4,4,1	171	6	6.23	0.34	1.21
Fe[3]	SNV−2,5,5,1	163	6	0.14	0.36	1.25

[1]sc−mt = scatter correction − mathematical treatment; n_{ext} = number of samples used to perform the external validation net of spectral outliers; SE_V = standard error of external validation; R^2_V = coefficient of determination of external validation; RPD = residual predictive deviation.

[2]isotypes G (IgG), A (IgA), and M (IgM) and their sum (IgTot).

[3]log-transformed.

[4]Detrend (d), Multiplicative scatter correction (MSC), No scatter correction (None), Standard normal variate (SNV), Standard normal variate+Detrend (SNVD).

of LV of the best prediction models ranged between 5 and 11 in cross-validation and between 2 and 10 in external validation. The most applied pre-treatment was multiplicative scatter correction for AA and standard normal variate for minerals, both preferring first rather than second order of derivatization. Most of the AA obtained good prediction accuracy when cross-validation was performed ($R^2_{CV} \geq 0.82$; Williams, 2003); in particular, Phe, Leu, Arg, and Thr reached a RPD ≥2.5 which represents the cut-off to consider a calibration model suitable for application in the field as a screening method (Williams, 2014). At the same time, it is worth considering that the conventional RPD classification is not adapted to the dairy sector. In fact, as reported by Grelet et al. (2021), even models showing RPD below 2.5 can be viewed as interesting. In dairy, the high cost of reference analyses and the difficulty of obtaining a high number of reference data should be considered when evaluating infrared prediction models.

Using milk, McDermott et al. (2016) predicted the Lys, Val, and Arg content via mid-infrared spectroscopy, which resulted in low correlations in cross-validation (0.69, 0.69, and 0.66, respectively). As expected, all AA suffered a slight reduction in accuracy when the models were applied to samples whose composition was masked. Thr, Phe, Arg, Leu, Trp, and His have maintained a level of accuracy sufficient to be used in a sample screening perspective (RPD ≥2), while the application of the equations for other AA is not recommended to be applied on external data sets.

Among minerals, only the equation for S achieved excellent precision in predicting the reference value which allows us to apply the model in quality control (R^2_{CV} = 0.93; RPD = 3.8). This is likely due to the presence of S in the structure of AA, making easy its identification with NIRS. In fact, only substances linked to organic molecules or associated to hydrated inorganic substances can be identified and predicted with infrared technologies (Clark et al., 1987). There-

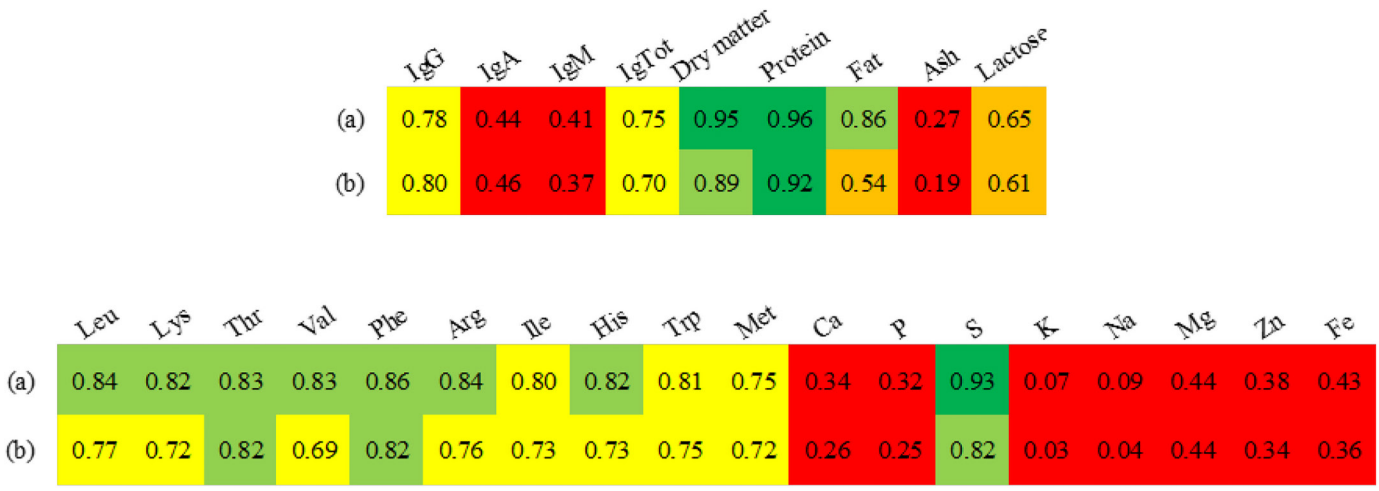

Figure 3. Traffic light classification[1] of predictive performance in (a) cross- and (b) external validation for the colostrum traits analyzed. [1] Based on ranges given by Williams (2003): coefficient of determination <0.50 (not recommended; red), 0.50-0.65 (exclusively for detection of extreme values/ comparison of groups; orange), 0.66-0.81 (approximate screening; yellow), 0.82-0.90 (good quantitative screening; light green), > 0.91 (excellent; dark green).

fore, minerals can be detected when they are found in organic complexes or chelates and this is the case of the sulfhydryl groups found in proteins (Büning-Pfaue, 2003). All the other minerals considered in the study obtained an insufficient prediction ($R^2_{CV} < 0.45$), which could again be related to the inorganic form or the low concentration in the samples. Soyeurt et al. (2009) obtained more accurate prediction models for Ca, P, K, Mg, and Na, being satisfactory for Ca and P ($R^2_{CV} > 0.82$), nevertheless they used milk spectra collected in the mid-infrared regions. Also, Visentin et al. (2016) predicted milk minerals content using mid-infrared spectroscopy without reaching successful accuracy ($R^2_{CV} \leq 0.62$). Performing the external validation minerals have maintained an unsatisfactory precision ($R^2_V < 0.45$), excepting for S which despite having undergone a reduction in accuracy, remains the only element that can still be estimated with the portable near-infrared spectrometer for screening ($R^2_V = 0.82$; RPD = 2.3). Figure 3 provides a visual representation of the accuracy changes for all the predicted traits between cross-validation (R^2_{CV}) and external validation (R^2_V) using a traffic light classification system. Residual of all prediction equations were normally distributed, and bias did not differ statistically from zero.

Although applications of portable NIRS instruments for the analysis of milk have been described in the literature (de la Roza-Delgado et al., 2017; Modroño et al., 2017), a direct comparison is not recommended as the spectral range on which the samples were scanned do not coincide due to the large number of tools present in the field or tested under experimental conditions. For instance, de la Roza-Delgado et al. (2017) collected spectra of raw milk from reflectance spectra between 1600 and 2400 nm, whereas Modroño et al. (2017) used a miniaturized spectrometer working in the range of 910–1676 nm. In any case, the ability of portable devices for BC quality discrimination and prediction of AA and minerals was investigated for the first time in the present study.

The procedure to evaluate the spectral ability to discriminate samples of good and low quality was carried out on the entire set net of outliers considering 3 different IgG concentrations, including the 50 g/L which is the concentration usually considered worldwide as the minimum for an adequate passive transfer of immunity in neonatal calves (Godden et al., 2019). The MCC calculated was equal to 0.25, 0.27, and 0.32 for IgG at 50, 60, and 70 g/L, respectively. In biochemistry, similar MCC values suggest that models are far from being considered as usable for punctual IgG prediction, however, it has to be considered that MCC ranges from −1 and 1, where values greater than 0 are indicative of a prediction in the correct direction (Chicco and Jurman, 2023). The confusion matrix which describes the classification performance of SCiO of the total number of samples is shown in Table 4 along with specificity and sensitivity which were equal to 61.33 and 74.48% for 50 g/L, 62.16 and 71.83% for 60 g/L, and 67.05 and 68.37 for 70 g/L. In particular, when setting the cut-off at 50 g/L the 'low quality' samples accounted for 12% of all samples and 4 wavelengths were retained, namely 740, 747, 939, and 1010 nm. In other words, 46 samples of 'low quality' and 426 samples of 'good quality' were correctly classified. This threshold, however, was quite strict for this study due to the low amount of 'low qual-

Table 4. Confusion matrix[1] for quality level (low vs high) defined using different cut-offs of IgG concentration (n = 647)

Quality	Cut-off					
Predicted	50 g/L		60 g/L		70 g/L	
Actual	Low	High	Low	High	Low	High
Low	*61.33%*	38.67%	*62.16%*	37.84%	*67.05%*	32.95%
	46	29	69	42	118	58
High	25.52%	*74.48%*	28.17%	*71.83%*	31.63%	*68.37%*
	146	426	151	385	149	322

[1]Percentage of samples correctly predicted are in the diagonal in italics.

ity' samples, with IgG below 50 g/L. Therefore, higher cut-offs were tested, i.e., at 60 and 70 g/L where the 'low quality' samples were 17 and 27%, respectively. When the threshold was set at 60 g/L, the wavelengths used were 740, 741, 939, and 1010 nm and the model correctly discriminates 62.2% of 'low quality' samples and 71.8% of the 'good quality' ones. The discriminant model developed using the third cut-off (70 g/L) retained a wavelength more (742 nm) compared with the previous cut-off and correctly identified 67.1 and 68.4% of the samples belonging to the 'low quality' and 'good quality' class, respectively. The spectral regions with important signals for IgG concentration were located in regions known for the presence of water, protein and fat (Šašić and Ozaki, 2001). Because absorption of these components overlap (Aernouts et al., 2015), achieving a precise correlation between the peak at a specific wavelength and the concentration of a BC component is not feasible.

The accuracy, which is the the overall proportion of samples correctly classified, was 68, 67, and 68% form the lowest to the highest threshold.

On-Farm Use

The ROC curves (Figure 4) demonstrate that SCiO predictions of IgG are very good for the classification of the quality of colostrum samples. The AUC values obtained using the external validation set are close to unity and indicate an excellent discriminant ability of the infrared-predicted IgG (Figure 4; Šimundić, 2009). For the less restrictive threshold, 70 g/L, the AUC was the lowest but still outperforming (0.911). As demonstrated by Chicco and Jurman (2023), even if both AUC and MCC are informative in classification issues, they provide different information. In this study, in fact, AUC looked as almost optimal (Figure 4) but the MCC calculated for the 3 IgG thresholds were rather far from 1 (perfect prediction), ranging from 0.25 to 0.37. Such a situation happens particularly when there

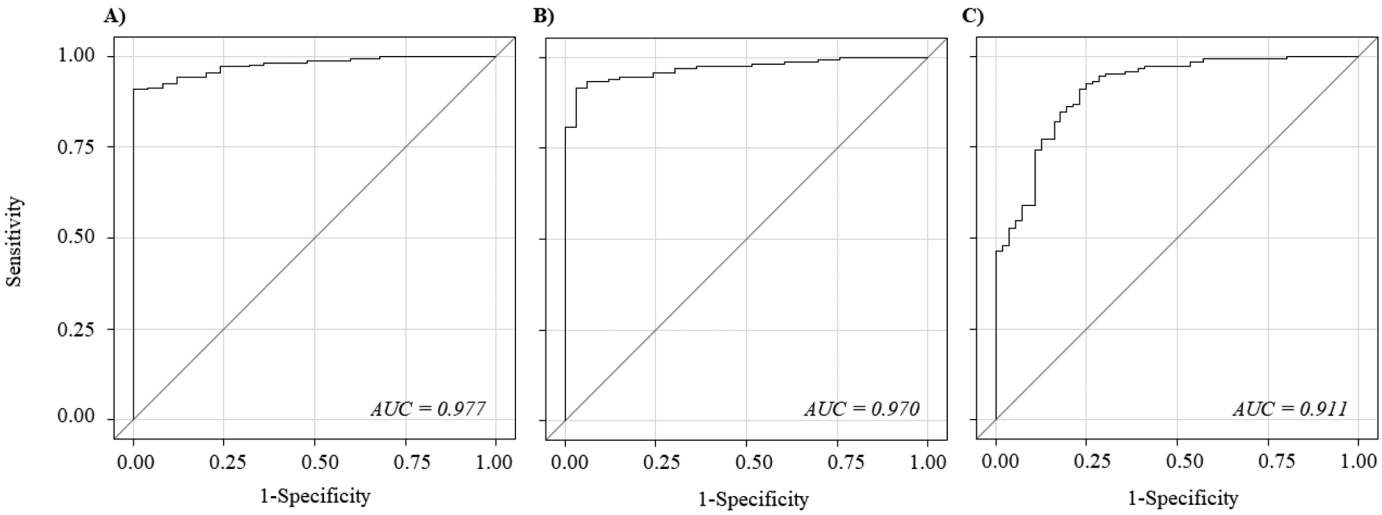

Figure 4. Receiver operating characteristic curves for the Ig G concentration predicted by the SCiO spectrometer along with the area under the curve (AUC). Thresholds used for 'low quality' samples classification were: A) 50, B) 60, and C) 70 g/L.

is an unbalance between the 2 classes, i.e., when a certain percentage of samples of the less represented class are misclassified. Although the effect of unbalanced classes is basically negligible for the AUC - which can still be very high and promising - it penalizes the MCC (Chicco and Jurman, 2023).

When used in the field, SCiO performance can be affected by factors not related to the goodness of fit of the models installed. For the analysis of BC, in fact, a brief protocol should be designed to ensure the quality of the analysis and of the predictions. Following specific guidelines can avoid undesired disturbances due to light, temperature, instrument cleanliness. Similar to other portable instruments, SCiO should be calibrated at the beginning of each analysis day, as indicated by the manufacturer, by taking a reading on a supplied ceramic white base that serves as a calibration blank sample. Given the portability, promising performance and cost, such a device opens the room for large scale studies on BC using data collected in the field by researchers, veterinarians, and farm managers.

CONCLUSIONS

In the present study, we attempted to predict the concentration of Ig isotypes, gross composition, minerals, and residual predictive deviation AA content in BC from spectra recorded using a hand-held wireless spectrometer operating in the near-infrared region. Although preliminary, results suggest that this technology has promising prediction performance for certain traits like IgG, IgTot, fat, and AA, while an excellent accuracy was obtained for dry matter, protein, and S in cross-validation. While the same traits were satisfactorily predicted in external validation, future emphasis could be placed on accounting for increased variability and validating models using samples from different farms. The good performance of the spectrometer for IgG punctual quantification, along with the ability to discriminate between good and low quality samples, represent an opportunity for dairy farmers. Similar hand-held devices can speed up a large-scale collection of data for targeted purposes, like selective breeding. As an example, a rapid assessment of the BC quality can be a useful driver to make considerations on the application and use in the farm but also in the food and pharmaceutical industry where BC is used as an ingredient. At the farm level, ensuring BC of appropriate quality to calves guarantee an optimal passive transfer of immunity.

ACKNOWLEDGMENTS

Authors acknowledge Dr Giulia Nardino and Dr Laura Posenato for the technical support during sampling, the personnel of the LaChi laboratory for the chemical analyses and the 9 farmers that joined the experiment.

REFERENCES

Aernouts, B., R. Van Beers, R. Watté, T. Huybrechts, J. Lammertyn, and W. Saeys. 2015. Visible and near-infrared bulk optical properties of raw milk. J. Dairy Sci. 98:6727–6738. https://doi.org/10.3168/jds.2015-9630.

Amr, M., Y. M. Sabry, and D. Khalil. 2018. Near-infrared optical MEMS spectrometer-based quantification of fat concentration in milk. 35th National Radio Science Conference (NRSC), Cairo, Egypt, 2018, pp. 409–416. https://doi.org/10.1109/NRSC.2018.8354389

AOAC International. 2000. Official Methods of Analysis. 17th ed. AOAC International, Gaithersburg, MD.

Beć, K. B., J. Grabska, and C. W. Huck. 2022. Miniaturized NIR Spectroscopy in Food Analysis and Quality Control: Promises, Challenges, and Perspectives. Foods 11:1465. https://doi.org/10.3390/foods11101465.

Beć, K. B., J. Grabska, H. W. Siesler, and C. W. Huck. 2020. Handheld near-infrared spectrometers: Where are we heading? NIR News 31:28–35. https://doi.org/10.1177/0960336020916815.

Blanco, M., and A. Peguero. 2010. Analysis of pharmaceuticals by NIR spectroscopy without a reference method. Trends Analyt. Chem. 29:1127–1136. https://doi.org/10.1016/j.trac.2010.07.007.

Büning-Pfaue, H. 2003. Analysis of water in food by near infrared spectroscopy. Food Chem. 82:107–115. https://doi.org/10.1016/S0308-8146(02)00583-6.

Chicco, D., and G. Jurman. 2023. The Matthews correlation coefficient (MCC) should replace the ROC AUC as the standard metric for assessing binary classification. BioData Min. 16:4. https://doi.org/10.1186/s13040-023-00322-4.

Clark, D. H., H. F. Mayland, and R. C. Lamb. 1987. Mineral analysis of forages with near infrared reflectance spectroscopy. Agron. J. 79:485–490. https://doi.org/10.2134/agronj1987.00021962007900030016x.

Costa, A., M. Franzoi, G. Visentin, A. Goi, M. De Marchi, and M. Penasa. 2021a. The concentrations of immunoglobulins in bovine colostrum determined by the gold standard method are genetically correlated with their near-infrared prediction. Genet. Sel. Evol. 53:87. https://doi.org/10.1186/s12711-021-00681-8.

Costa, A., A. Goi, M. Penasa, G. Nardino, L. Posenato, and M. De Marchi. 2021b. Variation of immunoglobulins G, A, and M and bovine serum albumin concentration in Holstein cow colostrum. Animal 15:100299. https://doi.org/10.1016/j.animal.2021.100299.

Costa, A., N. W. Sneddon, A. Goi, G. Visentin, L. M. E. Mammi, E. V. Savarino, F. Zingone, A. Formigoni, M. Penasa, and M. De Marchi. 2023. *Invited review:* Bovine colostrum, a promising ingredient for humans and animals - Properties, processing technologies, and uses. J. Dairy Sci. 106:5197–5217. https://doi.org/10.3168/jds.2022-23013.

Costa, A., G. Visentin, A. Goi, M. De Marchi, and M. Penasa. 2022. Genetic characteristics of colostrum refractive index and its use as a proxy for the concentration of immunoglobulins in Holstein cattle. Genet. Sel. Evol. 54:79. https://doi.org/10.1186/s12711-022-00768-w.

de la Roza-Delgado, B., A. Garrido-Varo, A. Soldado, A. González Arrojo, M. Cuevas Valdés, F. Maroto, and D. Pérez-Marín. 2017. Matching portable NIRS instruments for in situ monitoring indicators of milk composition. Food Control 76:74–81. https://doi.org/10.1016/j.foodcont.2017.01.004.

Dunn, A., A. Ashfield, B. Earley, M. Welsh, A. Gordon, and S. J. Morrison. 2017. Evaluation of factors associated with immunoglobulin G, fat, protein, and lactose concentrations in bovine colostrum and colostrum management practices in grassland-based dairy systems in Northern Ireland. J. Dairy Sci. 100:2068–2079. https://doi.org/10.3168/jds.2016-11724.

Elfstrand, L., H. Lindmark-Månsson, M. Paulsson, L. Nyberg, and B. Åkesson. 2002. Immunoglobulins, growth factors and growth hormone in bovine colostrum and the effects of processing. Int. Dairy J. 12:879–887. https://doi.org/10.1016/S0958-6946(02)00089-4.

Elsohaby, I., M. C. Windeyer, D. M. Haines, E. R. Homerosky, J. M. Pearson, J. T. McClure, and G. P. Keefe. 2018. Application of transmission infrared spectroscopy and partial least squares regression to predict immunoglobulin G concentration in dairy and beef cow colostrum. J. Anim. Sci. 96:771–782. https://doi.org/10.1093/jas/sky003.

Evangelista, C., L. Basiricò, and U. Bernabucci. 2021. An Overview on the Use of Near Infrared Spectroscopy (NIRS) on Farms for the Management of Dairy Cows. Agriculture 11:296. https://doi.org/10.3390/agriculture11040296.

Franzoi, M., A. Costa, A. Goi, M. Penasa, and M. De Marchi. 2022. Effectiveness of visible – Near infrared spectroscopy coupled with simulated annealing partial least squares analysis to predict immunoglobulins G, A, and M concentration in bovine colostrum. Food Chem. 371:131189. https://doi.org/10.1016/j.foodchem.2021.131189.

Godden, S. M. 2008. Colostrum management for dairy calves. Vet. Clin. North Am. Food Anim. Pract. 24:19–39. https://doi.org/10.1016/j.cvfa.2007.10.005.

Godden, S. M., J. E. Lombard, and A. R. Woolums. 2019. Colostrum Management for Dairy Calves. Vet. Clin. North Am. Food Anim. Pract. 35:535–556. https://doi.org/10.1016/j.cvfa.2019.07.005.

Goi, A., A. Costa, G. Visentin, and M. De Marchi. 2023a. Mid-infrared spectroscopy for large-scale phenotyping of bovine colostrum gross composition and immunoglobulins concentration. J. Dairy Sci. 106:6388–6401. https://doi.org/10.3168/jds.2022-23059.

Goi, A., M. De Marchi, and A. Costa. 2023. 2023b. Minerals and essential amino acids of bovine colostrum: phenotypic variability and predictive ability of mid- and near-infrared spectroscopy. J. Dairy Sci. on (Accepted).

Gopal, P. K., and H. S. Gill. 2000. Oligosaccharides and glycoconjugates in bovine milk and colostrum. Br. J. Nutr. 84(S1):69–74. https://doi.org/10.1017/S0007114500002270.

Grelet, C., P. Dardenne, H. Soyeurt, J. A. Fernandez, A. Vanlierde, F. Stevens, N. Gengler, and F. Dehareng. 2021. Large-scale phenotyping in dairy sector using milk MIR spectra: Key factors affecting the quality of predictions. Methods 186:97–111. https://doi.org/10.1016/j.ymeth.2020.07.012.

Kehoe, S. I., B. M. Jayarao, and A. J. Heinrichs. 2007. A survey of bovine colostrum composition and colostrum management practices on Pennsylvania dairy farms. J. Dairy Sci. 90:4108–4116. https://doi.org/10.3168/jds.2007-0040.

Llano Suárez, P., A. Soldado, A. González-Arrojo, F. Vicente, and B. de la Roza-Delgado. 2018. Rapid on-site monitoring of fatty acid profile in raw milk using a handheld near infrared sensor. J. Food Compos. Anal. 70:1–8. https://doi.org/10.1016/j.jfca.2018.03.003.

McDermott, A., G. Visentin, M. De Marchi, D. P. Berry, M. A. Fenelon, P. M. O'Connor, O. A. Kenny, and S. McParland. 2016. Prediction of individual milk proteins including free amino acids in bovine milk using mid-infrared spectroscopy and their correlations with milk processing characteristics. J. Dairy Sci. 99:3171–3182. https://doi.org/10.3168/jds.2015-9747.

Mishra, P., F. Marini, B. Brouwer, J. M. Roger, A. Biancolillo, E. Woltering, and E. Hogeveen-van Echtelt. 2021. Sequential fusion of information from two portable spectrometers for improved prediction of moisture and soluble solids content in pear fruit. Talanta 223:121733. https://doi.org/10.1016/j.talanta.2020.121733.

Modroño, S., A. Soldado, A. Martínez-Fernández, and B. de la Roza-Delgado. 2017. Handheld NIRS sensors for routine compound feed quality control: real time analysis and field monitoring. Talanta 162:597–603. https://doi.org/10.1016/j.talanta.2016.10.075.

Navrátilová, P., L. Hadra, M. Dračková, B. Janštová, L. Vorlová, and L. Pavlata. 2006. Use of FT-NIR Spectroscopy for Bovine Colostrum Analysis. Acta Vet. Brno 75:57–63. https://doi.org/10.2754/avb200675010057.

Playford, R. J., and M. J. Weiser. 2021. Bovine colostrum: Its constituents and uses. Nutrients 13:265. https://doi.org/10.3390/nu13010265.

Pu, Y., D. Pérez-Marín, N. O'Shea, and A. Garrido-Varo. 2021. Recent advances in portable and handheld NIR spectrometers and applications in milk, cheese and dairy powders. Foods 10:2377. https://doi.org/10.3390/foods10102377.

Puppel, K., M. Gołębiewski, G. Grodkowski, J. Slósarz, M. Kunowska-Slósarz, P. Solarczyk, M. Łukasiewicz, M. Balcerak, and T. Przysucha. 2019. Composition and Factors Affecting Quality of Bovine Colostrum: A Review. Animals (Basel) 9:1070. https://doi.org/10.3390/ani9121070.

Rivero, M. J., X. Valderrama, D. Haines, and D. Alomar. 2012. Prediction of immunoglobulin G content in bovine colostrum by near-infrared spectroscopy. J. Dairy Sci. 95:1410–1418. https://doi.org/10.3168/jds.2011-4532.

Ryckewaert, M., G. Chaix, D. Héran, A. Zgouz, and R. Bendoula. 2022. Evaluation of a combination of NIR micro-spectrometers to predict chemical properties of sugarcane forage using a multi-block approach. Biosyst. Eng. 217:18–25. https://doi.org/10.1016/j.biosystemseng.2022.02.019.

Santos, P. M., E. R. Pereira-Filho, and L. E. Rodriguez-Saona. 2013. Application of Hand-Held and Portable Infrared Spectrometers in Bovine Milk Analysis. J. Agric. Food Chem. 61:1205–1211. https://doi.org/10.1021/jf303814g.

Šašić, S., and Y. Ozaki. 2001. Short-wave near-infrared spectroscopy of biological fluids. 1. Quantitative analysis of fat, protein, and lactose in raw milk by partial least-squares regression and band assignment. Anal. Chem. 73:64–71. https://doi.org/10.1021/ac000469c.

Šimundić, A. 2009. Measures of diagnostic accuracy: basic definitions. EJIFCC 19:203.

Sørensen, L. K. 2002. True accuracy of near infrared spectroscopy and its dependence on precision of reference data. J. Near Infrared Spectrosc. 10:15–25. https://doi.org/10.1255/jnirs.317.

Soyeurt, H., D. Bruwier, J.-M. Romnee, N. Gengler, C. Bertozzi, D. Veselko, and P. Dardenne. 2009. Potential estimation of major mineral contents in cow milk using mid-infrared spectrometry. J. Dairy Sci. 92:2444–2454. https://doi.org/10.3168/jds.2008-1734.

Sun, Y., Y. Wang, J. Huang, G. Ren, J. Ning, W. Deng, L. Li, and Z. Zhang. 2020. Quality assessment of instant green tea using portable NIR spectrometer. Spectrochim. Acta Part A Mol. Spectrochim. Acta A Mol. Biomol. Spectrosc. 240:118576. https://doi.org/10.1016/j.saa.2020.118576.

VDLUFA. 2013. Handbuch der landwirtschaftlichen Versuchs-und Untersuchungsmethodik, Methodenbuch Band VI–Chemische, physikalische und mikrobiologische Untersuchungsverfahren für Milch Milchprodukte und Molkereihilfsstoffe. VDLUFA-Verlag, Darmstadt, Germany.

Visentin, G., M. Penasa, P. Gottardo, M. Cassandro, and M. De Marchi. 2016. Predictive ability of mid-infrared spectroscopy for major mineral composition and coagulation traits of bovine milk by using the uninformative variable selection algorithm. J. Dairy Sci. 99:8137–8145. https://doi.org/10.3168/jds.2016-11053.

Wang, Y., Q. Liu, H. Hou, S. Rho, B. Gupta, Y. Mu, and W. Shen. 2018. Big data driven outlier detection for soybean straw near infrared spectroscopy. J. Comput. Sci. 26:178–189. https://doi.org/10.1016/j.jocs.2017.06.008.

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. 5.0 ed. PDK Grain, Nanaimo, BC, Canada.

Williams, P. 2014. The RPD statistic: A tutorial note. NIR News 25:22–26. https://doi.org/10.1255/nirn.1419.

Williams, P. C. 2003. Near-infrared technology getting the best out of light. A short course in the practical implementation of near-infrared spectroscopy for the user (1.1 ed.), PDK Projects Inc, Nanaimo, Canada. P. 109.

ORCIDS

Arianna Goi https://orcid.org/0000-0003-3341-9775
Angela Costa https://orcid.org/0000-0001-5353-8988
Massimo De Marchi https://orcid.org/0000-0001-7814-2525