



J. Dairy Sci. 100:1–12  
<https://doi.org/10.3168/jds.2017-12720>  
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## Standardization of milk mid-infrared spectrometers for the transfer and use of multiple models

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### ABSTRACT

An increasing number of models are being developed to provide information from milk Fourier transform mid-infrared (FT-MIR) spectra on fine milk composition, technological properties of milk, or even cows' physiological status. In this context, and to take advantage of these existing models, the purpose of this work was to evaluate whether a spectral standardization method can enable the use of multiple equations within a network of different FT-MIR spectrometers. The piecewise direct standardization method was used, matching “slave” instruments to a common reference, the “master.” The effect of standardization on network reproducibility was assessed on 66 instruments from 3 different brands by comparing the spectral variability of the slaves and the master with and without standardization. With standardization, the global Mahalanobis distance from the slave spectra to the master spectra was reduced on average from 2,655.9 to 14.3, representing a significant reduction of noninformative spectral variability. The transfer of models from instrument to instrument was tested using 3 FT-MIR models predicting (1) the quantity of daily methane emitted by dairy cows, (2) the concentration of polyunsaturated fatty acids in milk, and (3) the fresh cheese yield. The differences, in terms of root mean squared error, between master predictions and slave predictions were reduced after standardization on average from 103 to 17 g/d, from 0.0315 to 0.0045 g/100 mL of milk, and from 2.55 to 0.49 g of curd/100 g of milk, respectively. For all the models, standard deviations of predictions among all the instruments were also reduced by 5.11 times for methane, 5.01 times for polyunsaturated fatty acids, and 7.05 times for fresh cheese yield, showing an improvement of prediction reproducibility within

the network. Regarding the results obtained, spectral standardization allows the transfer and use of multiple models on all instruments as well as the improvement of spectral and prediction reproducibility within the network. The method makes the models universal, thereby offering opportunities for data exchange and the creation and use of common robust models at an international level to provide more information to the dairy sector from direct analysis of milk.

**Key words:** Fourier transform mid-infrared spectra, standardization, milk, model transfer

### INTRODUCTION

Over the past decade, the number of research studies seeking to extract more quantitative information from the Fourier transform mid-infrared (FT-MIR) spectra has increased constantly (De Marchi et al., 2014). Equations based on the full spectrum have been developed for the determination of fine milk components such as fatty acid profiles (Soyeurt et al., 2006; Rutten et al., 2009), protein composition (Bonfatti et al., 2011), minerals (Soyeurt et al., 2009), ketone bodies (van Kneegsel et al., 2010), citrate (Grelet et al., 2016), and lactoferrin (Soyeurt et al., 2007). Other studies have focused on FT-MIR spectra to build equations predicting technological properties of milk such as milk acidity (De Marchi et al., 2009), ability to coagulate, firmness of curd, or cheese yield (Dal Zotto et al., 2008; Colinet et al., 2015). Recent work has directly considered the FT-MIR spectrum of milk as a reflection of cows' status, with FT-MIR equations being developed to predict methane emissions of dairy cows (Dehareng et al., 2012; Vanlierde et al., 2016), likelihood of conception (Hempstalk et al., 2015), body energy status (McParland et al., 2011), energy intake and efficiency (McParland et al., 2014). In the work of Lainé et al. (2017), the spectrum is even considered as a response for which the effect of pregnancy is evaluated. Hence, the FT-MIR analysis of milk allows the measurement

Received February 13, 2017.

Accepted June 5, 2017.

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of multiple variables to be used for fine milk quality control in industry, management of herds, or the generation of new phenotypes for genetic studies. Even if some models could be statistically considered as low quality, they are of major interest for the dairy sector because they provide the opportunity to predict key variables that were not available before on a large scale and in a cost-effective way.

However, developing such models is time consuming and expensive given that they require the analysis of a large number of samples to cover the whole distribution of the studied trait as well as a large spectral variability. Therefore, there is a clear interest in sharing predictive models among milk laboratories and milk recording organizations. However, a major issue with FT-MIR data is related to the specific instrumental response produced by each spectrometer. These differences between spectral responses of instruments originate from the physical characteristics and acquisition modes specific to each model of machine and from the different uses, piece replacements, and maintenance operations specific to each spectrometer. Differences in spectral response cause difficulties in combining spectra as well as bias in predictions when transferring a calibration model built on one instrument to another instrument. Consequently, exchanges of data and models are limited. To cope with this issue, classical models predicting the main milk components by FT-MIR (e.g., fat and proteins) are monitored and adjusted over instruments and over time using slope and intercept correction. The method is based on the adjustment of the models according to interlaboratory study samples, in which the content of the relevant components is known. However, for most of the new predicted variables (e.g., cows' physiological status or hard-to-measure fine milk components), it is expensive or almost impossible to produce interlaboratory study samples with a known content of the variable of interest. This makes it difficult or impossible to adjust a model after transfer to another spectrometer. Consequently, a model developed on one instrument theoretically can be used only by that instrument because of its specific format. In the context of increasing interest in using new models, the impossibility of transferring them leads to a suboptimal situation, as the creation of robust models is difficult and expensive.

For this reason, it is necessary to implement a preliminary step of spectral standardization permitting the sharing of models. In the context of projects involving international networking, since December 2011 a large instrument standardization network has been developed to harmonize the format of FT-MIR milk spectral response. The objective is to clear the way for potential collaborations between organizations using

FT-MIR spectrometers for milk analysis. The possibility of creating common data sets and common models that can be transferred from laboratory to laboratory and used by all instruments allows financial and technical resources to be pooled. Moreover, the possibility of merging spectral data, as far as the reference methods are comparable, allows the inclusion of different feeding systems, breeds, and management, thus increasing the robustness of the developed common models. Over the years the network size has increased, and as many as 127 instruments of 3 different brands coming from 14 countries on 4 continents (North America, Asia, Europe, and Oceania) have been standardized. Recently, it has been shown that using the piecewise direct standardization (**PDS**) method it is possible to transfer a high-quality fat model from one instrument to more than 20 different instruments in the network (Grelet et al., 2015). However, there is no information about the possibility of transferring models with lower accuracy or predicting fine milk composition or indirect variables, which are not milk components and consequently are predicted indirectly, despite the fact that these models are of great interest to the dairy sector. Furthermore, the effects of standardization on spectral and prediction reproducibility over the network have never been assessed even though it is essential for management or breeding purposes. Therefore, the objectives of this study were to evaluate the effect of the PDS standardization method (1) on spectral reproducibility over spectrometers in a network, (2) on transferring multiple and varied FT-MIR models from one instrument to another, and (3) on the accuracy and reproducibility of predictions among all apparatus. The global perspective is to make all spectrometers speak the same language, thereby allowing the transfer and exchange of developed models predicting classical and new parameters throughout the network.

## MATERIALS AND METHODS

### *Instrumentation*

The different instruments available through the network are FT 6000, FT+, FT2, and FT120 (Foss, Hillerød, Denmark); FTS (Bentley, Chaska, MN); and Standard Lactoscope FT-MIR automatic (Delta Instruments, Drachten, the Netherlands). The wave number ranges of the different brands were 925.66 to 5,010.15  $\text{cm}^{-1}$  for Foss instruments, 649.03 to 3,998.59  $\text{cm}^{-1}$  for Bentley instruments, and 397.31 to 4,000  $\text{cm}^{-1}$  for Delta instruments. The resolution used was 8  $\text{cm}^{-1}$  for Delta and Bentley instruments and unknown for Foss instruments. As the goal of this work was to validate the standardization method rather than to compare

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