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Effectiveness of mid-infrared spectroscopy to predict fatty acid composition of Brown Swiss bovine milk

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*Mid-infrared spectroscopy (MIR) is used to predict fatty acid (FA) composition of individual milk samples (*n *= 267) of Brown Swiss cows. FAs were analyzed by gas chromatography as a reference method. Samples were scanned (4000 to 900 cm^{-1}) by MIR, and predictive models were developed using modified partial least squares regressions with full cross-validation. The methods using a first derivative or multiplicative scatter corrected plus first derivative resulted, on average, in the best predictions. Coefficients of correlation between measured and predicted C8:0, C10:0, C12:0, C14:0, anteiso-C17:0, c9-C18:1, and medium- and long-chain FA, and saturated, monounsaturated and unsaturated FA ranged from 0.71 to 0.77, suggesting that prediction models can be implemented in milk recording schemes to routinely collect information on FA composition from the whole Brown Swiss population for breeding purposes.*

Keywords: bovine milk, fatty acid, mid-infrared spectroscopy, Brown Swiss

Implication

Mid-infrared spectroscopy demonstrated the potential to predict fatty acid (FA) composition by non-destructive, low cost and fast analysis. The prediction models were able to identify high and low values of individual and groups of FA in milk. Models developed in this study might be used in Brown Swiss population breeding programs aimed at improving the value of milk for human health and nutrition.

Introduction

Milk fat is a mix of glycerides, complex lipids and liposoluble substances, and the main components (96% to 98%) are the triglycerides (Jensen, 2002). According to their saturation, fatty acids (FAs) are classified as saturated (SFA), monounsaturated (MUFA) and polyunsaturated (PUFA). Fat of bovine milk is composed of 70% SFA, 25% MUFA and 5% PUFA (Grummer, 1991; Shingfield *et al.*, 2003).

Milk quality aspects are gaining interest among consumers, particularly those related to human health. The SFA increase blood cholesterol, which in turn is associated with increased cardio-vascular diseases, risk of obesity, atherosclerosis and coronary heart diseases (Mensink and Katan, 1992; German *et al.*, 2009), whereas the unsaturated FA (UFA) reduce the level of cholesterol in blood (Haug *et al.*, 2007); among them, PUFA decrease the cholesterol content more strongly than MUFA (Williams, 2000). In addition, milk fat is the major source of conjugated linoleic acid (CLA; *c*9,*t*11-C18:2) in human diet, accounting for 70% of total daily CLA intake (Bauman *et al.*, 2005). Experimental evidences suggest that CLA may have anticarcinogenic, antiatherosclerotic, antidiabetic and immunomodulating effects (Bhattacharya *et al.*, 2006). Because of the relevance of milk fat on health aspects, it would be interesting to enhance the production of favorable FA through feeding of cows (Chilliard and Ferlay, 2004; Mele, 2009) and breeding (Arnould and Soyeurt, 2009).

Several studies estimated genetic variation of FA (Soyeurt *et al.*, 2007; Stoop *et al.*, 2008; Mele *et al.*, 2009) but gas chromatography (GC) is an expensive and time-consuming analysis; hence, a rapid method to determine FA in milk is crucial to extend the collection of phenotypic records at the population level.

Mid-infrared spectroscopy (MIR) is widely used in official milk recording schemes to determine the chemical composition of milk (Lynch *et al.*, 2006). Its potential has also been demonstrated to predict coagulation properties of bovine milk (Dal Zotto *et al.*, 2008; De Marchi *et al.*, 2009b), detail milk protein composition (De Marchi *et al.*, 2009a) and

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acetone content for the detection of subclinical ketosis (Heuer *et al*., 2001). Soyeurt *et al*. (2006) and Rutten *et al*. (2009) demonstrated the accuracy of the prediction of FA composition using MIR, but only for the most representative FA. Recently, Coppa *et al*. (2010) reported that near-infrared spectroscopy might be used to predict FA of oven-dried milk, whereas less satisfactory results are obtained for liquid milk.

The aim of this research was to predict individual and selected categories of FA of bovine milk using MIR.

Material and methods

Sample collection

Samples used for GC analysis ($n = 267$) were randomly selected from 1200 Italian Brown Swiss cows involved in a wide research project conducted in northern Italy from June 2006 to July 2007 (for details, see Cecchinato *et al*., 2009). Briefly, the project was based on the collection of individual milk samples from cows of different parity and stage of lactation, progeny of 50 AI sires, and reared in 30 herds located in the plain, hill and mountain. Herds largely differed in terms of feeding systems, particularly when comparing those from mountain and plain. The later used mainly silages and concentrates, whereas the former were mainly based on hay and fewer concentrates. After collection, samples destined to GC analysis were stored at −20°C without any preservative and transferred to the milk quality laboratory of the University of Pisa (Pisa, Italy).

FA analysis

Milk fat was extracted according to Mele *et al*. (2009). Methyl esters of medium- and long-chain FA were prepared by the alkali-catalyzed *trans*-methylation procedure in Christie (1982) with C9:0 and C23:0 methyl esters (Sigma Chemical Co., St. Louis, MO) as the internal standards. FA composition was determined by GC using a ThermoQuest (Milan, Italy) gas chromatograph equipped with a flame ionization detector and a high polar fused silica capillary column (Chrompack CP-Sil 88 Varian, Middelburg, the Netherlands; 100 m × 0.25 mm i.d.; film thickness 0.20 μm). Helium was used as the carrier gas at a flow of 1 ml/min. The split ratio was 1 : 100. An aliquot of the sample was injected under the following GC conditions: the oven temperature was programmed at 60°C and held for 4 min, then increased to 120°C at a rate of 10°C/min, held for 1 min, increased to 180°C at a rate of 2°C/min, held for 18 min, increased to 200°C at a rate of 2°C/min, held for 1 min, increased at 230°C at a rate of 5°/min and maintained at this temperature for 19 min. The injector temperature was set at 270°C, whereas the detector temperature was at 300°C. Individual FA methyl esters were identified by comparing them with a standard mixture of 52 Component FAME Mix (Nu-Chek Prep, Inc., Elysian, MN, USA), and the identification of C18:1 isomers was based on a commercial standard mixture (Supelco, Bellefonte, PA, USA) and on chromatograms published by Kramer *et al*. (2008). All the methods that used peak normalization and that expressed results as a relative percentage of the area of the analyzed peaks were subject to overestimation because the small peak areas were not considered. To avoid this problem, two internal standards were used: C9:0 for FA from C:4 to C:13 and C23:0 for FA from C:14 to C:24. Milk FA composition was determined by GC and expressed as g/kg of milk. For each FA, response factors to flame ionization detector and inter- and intra-assay coefficients of variation were calculated by using a reference standard butter (CRM 164, Community Bureau of Reference, Brussels, Belgium). Intra-assay coefficients of variation ranged from 0.5% to 1.5%, whereas inter-assay coefficients of variation ranged from 1.5% to 2.5%.

Only major FA with carbon chain no longer than 20 and categories of FA were studied. In particular, FA were grouped according to either the length of the carbon chain: medium-chain FA (MCFA; from C11 to C17); long-chain FA (LCFA; from C18 to C22); or to the saturation degree: SFA; MUFA; PUFA; UFA; or to the characteristics of the carbon chain: branched-chain FA (BCFA; iso-14:0, anteiso-C15:0, iso-C16:0, anteiso-C17:0); trans FA (TFA; *t*6,8-C18:1, *t*9-C18:1, *t*10-C18:1, *t*11-C18:1, *t*12-C18:1,*c*9,*t*11-C18:2).

Mid-infrared spectra acquisition and multivariate data analysis

Mid-infrared spectra were collected on the day of sampling in the Food Lab of the Department of Animal Science (University of Padova) from 0.25 ml of milk over the spectral range of 4000 to 900 cm^{-1} using a Milko-Scan FT120 (Foss Electric A/S, Hillerød, Denmark). Duplicate spectra were captured for each individual sample using the calibration mode and averaged before data analysis. Principal component analysis (PCA) and partial least squares (PLS) regressions were carried out through the Unscrambler software (version 9.6; Camo A/S, Oslo, Norway), and a new smaller set of variables called principal components and loadings (L#) were obtained. A graphical representation of similarities and differences between spectra was derived from PCA; this allowed the identification of possible outliers in the spectral data set (Martens and Naes, 1989). Prediction models were computed by PLS regression and confirmed using full cross-validation, and prediction residuals were combined to calculate the root mean square error of cross-validation ($RMSE_{CV}$; Hubert and Vanden Branden, 2003). Besides the untreated spectra, two mathematical treatments were tested: first derivative (Savitzky-Golay, three data points each side) and multiplicative scatter corrected (MSC) plus first derivative (Savitzky-Golay, three data points each side) spectra. The accuracy of the prediction models was evaluated using $RMSE_{CV}$, the correlation coefficient in cross-validation (r_{CV}) and the optimum number of L# (Hubert and Vanden Branden, 2003).

The range error ratio (RER), calculated as the ratio between the range and the $RMSE_{CV}$ of the parameter (Williams, 2001), was used to test the practical utility of the prediction models. RER is a method of standardizing the $RMSE_{CV}$ by relating it to the range of the reference data. For example, RER values of less than six indicate very poor classification and are not recommended for any application;

RER values between 7 and 20 classify the model as poor to fair and indicate that the model could be used in a screening application; and RER values between 21 and 30 indicate a good classification suggesting that the model would be suitable for a role in a quality control application (Williams, 2001). However, calibrations with lower statistical performance may still be useful depending on the accuracy required in field conditions.

Results

FA composition

Mean, standard deviation (s.d.), coefficient of variation (CV) and range of individual FA and of selected categories are presented in Tables 1 and 2. The C16:0 (10.52 g/kg) and *c*9-C18:1 (6.81 g/kg) were the major FA in milk, followed by C14:0 (4.27 g/kg) and C18:0 (3.28 g/kg). As expected, SFA represented the prevalent fraction (21.84 g/kg), followed by MCFA (19.00 g/kg) and LCFA (12.82 g/kg). All FA and selected categories showed large variability with CV that ranged from 0.21 (C16:0) to 0.47 (iso-C14:0) for individual FA (Table 1), and from 0.20 (SFA) to 0.28 (TFA) for groups of FA (Table 2).

MIR spectra

Figure 1 shows an example of MIR spectrum. A portion of the spectrum was truncated before the analysis due to its low signal-to-noise ratio (Pillonel *et al*., 2003); two spectra regions (3470 to 3040 cm^{-1} and 1700 to 1600 cm^{-1}) were omitted from PLS analysis. The high level of noise at these wavelengths may be the consequence of the absorption of water in the spectral regions (Hewavitharana and Brakel, 1997; Jørgensen and Næs, 2004). The principal MIR regions used to estimate FA composition of milk were located between 1736 and 1805 cm^{-1} and between 2823 and 3016 cm^{-1}. Coates (2000) and Lefèvre and Subirade (2000) indicated that 1745, 2928 and 2855 cm^{-1} are the frequencies correlated with the vibration of the FA carbonyl group. The wavenumbers between approximately 1050 and 1600 cm^{-1} are associated with several specific chemical bonds such as C–H bending (1493 cm^{-1}) and C–O stretching. PCA of the untreated spectra allowed for the investigation of the influence plot and hence the identification of possible outliers.

Prediction models

Tables 3 and 4 summarized the $RMSE_{CV}$, r_{CV}, L# and RER of each calibration equation built from spectra and FA contents. Prediction models were developed using spectra in several forms: untreated, first derivative and MSC plus first derivative giving three models for each predicted trait. A normalized and second derivative pre-treatment offered no improvement of prediction; hence, these results are not reported. The $RMSE_{CV}$, r_{CV} and L# were used to compare

Table 1 *Descriptive statistics of individual FA (expressed in g/kg of milk) determined by GC analysis*

FA	Mean	s.d.	CV	Range
C8:0	0.41	0.11	0.26	0.15 to 0.85
C10:0	1.09	0.30	0.28	0.34 to 2.28
C12:0	1.36	0.39	0.29	0.40 to 2.90
iso-C14:0	0.04	0.02	0.47	0.01 to 0.10
C14:0	4.27	0.95	0.22	1.42 to 7.56
C14:1-*c*9	0.35	0.11	0.33	0.10 to 0.73
anteiso-C15:0	0.17	0.04	0.24	0.06 to 0.32
C15:0	0.37	0.10	0.27	0.15 to 0.73
iso-C16:0	0.09	0.03	0.37	0.03 to 0.18
C16:0	10.52	2.23	0.21	3.41 to 15.85
C16:1-*c*9	0.44	0.15	0.34	0.14 to 1.00
anteiso-C17:0	0.06	0.02	0.35	0.01 to 0.12
C17:0	0.15	0.03	0.23	0.06 to 0.29
C18:0	3.28	1.06	0.32	0.75 to 7.85
*t*6,8-C18:1	0.08	0.02	0.33	0.02 to 0.16
*t*9-C18:1	0.10	0.03	0.25	0.04 to 0.17
*t*10-C18:1	0.16	0.06	0.38	0.04 to 0.60
*t*11-C18:1	0.34	0.11	0.33	0.09 to 0.84
*t*12-C18:1	0.14	0.04	0.27	0.04 to 0.27
*c*9-C18:1	6.81	1.70	0.25	2.61 to 12.55
*c*11-C18:1	0.15	0.06	0.37	0.05 to 0.37
*c*12-C18:1	0.16	0.04	0.29	0.05 to 0.31
*c*6-C18:2	0.84	0.20	0.24	0.35 to 1.47
*c*9,*t*11-C18:2	0.18	0.05	0.30	0.05 to 0.38
C18:3n-3	0.16	0.06	0.41	0.05 to 0.46
C20:0	0.03	0.01	0.33	0.01 to 0.10

FA = fatty acids; GC = gas chromatography; CV = coefficient of variation.

Table 2 *Descriptive statistics of FA categories (expressed in g/kg of milk) determined by GC analysis*

FA category	Mean	s.d.	CV	Range
MCFA	19.00	3.95	0.21	6.34 to 30.63
LCFA	12.82	3.07	0.24	5.26 to 23.22
SFA	21.84	4.28	0.20	7.61 to 31.47
MUFA	8.91	2.07	0.23	3.41 to 15.44
PUFA	1.35	0.30	0.22	0.55 to 2.22
UFA	10.26	2.29	0.22	3.99 to 17.32
BCFA	0.36	0.09	0.26	0.13 to 0.64
TFA	0.84	0.23	0.28	0.22 to 1.65

FA = fatty acids; GC = gas chromatography; CV = coefficient of variation; MCFA = medium-chain FA; LCFA = long-chain FA; SFA = saturated FA; MUFA = monounsaturated FA; PUFA = polyunsaturated FA; UFA = unsaturated FA; BCFA = branched-chain FA; TFA = trans FA.

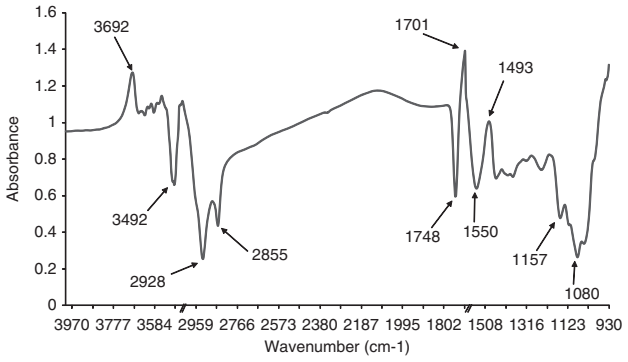

Figure 1 Example of algorithm unprocessed MIR spectrum for milk.

Table 3 *PLS predictions for individual FA (expressed in g/kg of milk) using untreated and pretreated mid-infrared spectra (preferred model in bold)*

	Untreated data				First derivative[a]				MSC + first derivative			
FA	$RMSE_{CV}$	r_{CV}	L#	RER	$RMSE_{CV}$	r_{CV}	L#	RER	$RMSE_{CV}$	r_{CV}	L#	RER
C8:0	0.07	0.69	6	9.51	0.07	0.71	6	9.96	**0.07**	**0.74**	**6**	**10.10**
C10:0	0.20	0.72	10	9.63	0.20	0.73	7	9.80	**0.19**	**0.73**	**7**	**10.10**
C12:0	0.26	0.72	9	9.65	**0.25**	**0.75**	**7**	**10.08**	0.25	0.74	7	9.90
iso-C14:0	**0.01**	**0.56**	**5**	**6.57**	0.01	0.50	5	6.26	0.01	0.48	4	6.49
C14:0	0.62	0.75	10	9.97	**0.60**	**0.77**	**6**	**10.23**	0.64	0.72	7	9.55
C14:1-*c*9	0.08	0.66	12	7.55	**0.08**	**0.68**	**7**	**7.81**	0.08	0.64	5	7.77
anteiso-C15:0	0.03	0.60	5	7.62	**0.03**	**0.64**	**5**	**7.91**	0.03	0.64	6	8.15
C15:0	0.08	0.62	11	7.76	**0.07**	**0.63**	**7**	**7.85**	0.08	0.56	5	7.51
iso-C16:0	0.03	0.53	5	5.88	0.03	0.52	4	5.73	**0.03**	**0.58**	**8**	**6.04**
C16:0	**1.59**	**0.70**	**8**	**7.82**	1.63	0.68	6	7.62	1.67	0.67	7	7.46
C16:1-*c*9	0.11	0.57	7	7.54	**0.11**	**0.60**	**5**	**7.77**	0.11	0.60	5	7.81
anteiso-C17:0	0.01	0.73	12	8.02	**0.01**	**0.73**	**7**	**8.10**	0.01	0.72	5	7.91
C17:0	**0.03**	**0.56**	**2**	**8.39**	0.03	0.55	2	8.31	0.03	0.49	1	7.64
C18:0	**0.75**	**0.65**	**9**	**9.48**	0.74	0.66	6	9.55	0.74	0.66	6	9.53
*t*6,8-C18:1	0.02	0.49	4	6.85	**0.02**	**0.59**	**6**	**7.55**	0.02	0.55	6	7.29
*t*9-C18:1	0.02	0.60	4	6.57	**0.02**	**0.63**	**5**	**6.73**	0.02	0.62	6	6.63
*t*10-C18:1	0.05	0.46	14	10.49	0.05	0.48	9	10.58	**0.04**	**0.51**	**7**	**14.60**
*t*11-C18:1	0.09	0.51	5	8.02	0.09	0.54	6	8.21	**0.09**	**0.56**	**6**	**8.01**
*t*12-C18:1	0.03	0.48	4	6.78	0.03	0.55	4	7.33	**0.03**	**0.63**	**5**	**8.01**
*c*9-C18:1	1.17	0.71	8	8.47	1.14	0.73	7	8.68	**1.13**	**0.73**	**7**	**8.80**
*c*11-C18:1	0.04	0.59	14	7.48	0.04	0.57	7	7.37	**0.04**	**0.59**	**8**	**7.56**
*c*12-C18:1	0.04	0.40	7	6.15	0.04	0.38	6	6.09	**0.04**	**0.52**	**6**	**7.12**
*c*6-C18:2	0.74	0.50	6	1.52	**0.17**	**0.54**	**5**	**6.64**	0.17	0.50	4	6.41
C18:3n-3	0.05	0.48	8	8.55	0.05	0.49	6	8.58	**0.04**	**0.51**	**5**	**10.34**
C20:0	0.01	0.51	9	9.27	0.01	0.53	5	9.47	**0.01**	**0.54**	**6**	**9.78**
*c*9,*t*11-C18:2	0.05	0.46	7	7.27	0.05	0.45	7	7.42	**0.04**	**0.58**	**7**	**8.23**

PLS = partial least squares; FA = fatty acids; MSC = multiplicative scatter correction; $RMSE_{CV}$ = root mean square error of cross-validation; r_{CV} = coefficient of correlation of cross-validation; L# = number of partial least squares loadings; RER = range error ratio.
[a]Savitzky–Golay, three data points each side.

Table 4 *PLS predictions for FA categories (expressed in g/kg of milk) using untreated and pretreated mid-infrared spectra (preferred model in bold)*

	Untreated data				First derivative[a]				MSC + first derivative			
FA category	$RMSE_{CV}$	r_{CV}	L#	RER	$RMSE_{CV}$	r_{CV}	L#	RER	$RMSE_{CV}$	r_{CV}	L#	RER
MCFA	2.71	0.72	11	8.96	**2.66**	**0.73**	**6**	**9.15**	2.66	0.73	7	9.12
LCFA	2.18	0.70	6	8.24	2.03	0.73	6	8.83	**1.94**	**0.76**	**6**	**9.27**
SFA	3.15	0.69	5	7.70	**2.97**	**0.72**	**6**	**8.06**	3.36	0.66	6	7.16
MUFA	1.56	0.64	1	7.69	**1.39**	**0.74**	**7**	**8.62**	1.50	0.68	5	7.99
PUFA	0.25	0.55	5	6.82	0.24	0.59	5	7.09	**0.22**	**0.64**	**5**	**7.66**
UFA	1.79	0.62	6	7.45	1.73	0.66	5	7.72	**1.57**	**0.71**	**5**	**8.51**
BCFA	0.08	0.58	6	6.79	**0.07**	**0.68**	**6**	**7.60**	0.07	0.63	5	7.39
TFA	0.19	0.56	5	7.43	0.19	0.59	5	7.60	**0.18**	**0.63**	**6**	**7.93**

PLS = partial least squares; FA = fatty acids; MSC = multiplicative scatter correction; $RMSE_{CV}$ = root mean square error of cross-validation; r_{CV} = coefficient of correlation of cross-validation; L# = number of partial least squares loadings; RER = range error ratio; MCFA = medium-chain FA; LCFA = long-chain FA; SFA = saturated FA; MUFA = monounsaturated FA; PUFA = polyunsaturated FA; UFA = unsaturated FA; BCFA = branched-chain FA; TFA = trans FA.
[a]Savitzky–Golay, three data points each side.

models for accuracy. If two models produced similar results for a given trait, the preferred model was that with the lowest $RMSE_{CV}$, the highest r_{CV} and the lowest number of L#.

Prediction models were calculated using FA concentration in milk and FA concentration in fat as reference data. Overall, the pre-treated MIR spectra with first derivative or MSC plus first derivative gave the best results. The PLS method using untreated spectra provided good outcomes only for the prediction of iso-C14:0, C16:0, C17:0 and C18:0.

The r_{CV} of FA ranged from 0.51 (*t*10-C18:1 and C18:3n-3) to 0.77 (C14:0) for individual FA (Table 3), and from 0.63 (TFA) to 0.76 (LCFA) for groups of FA. Williams (2003) suggested

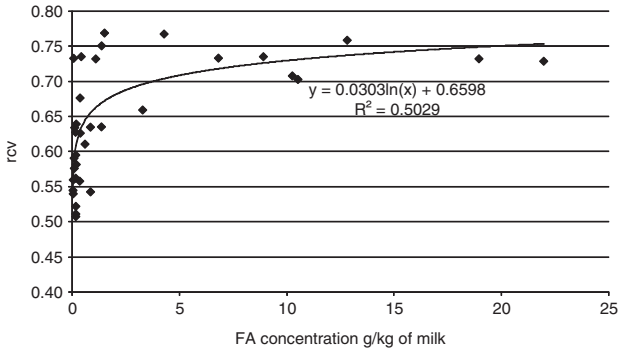

Figure 2 Relationship between fatty acids (expressed in g/kg of milk) and modeling success expressed as g/kg *v.* r_{CV} (coefficient of correlation of cross-validation).

that r_{CV} between 0.70 and 0.80 indicate that discrimination between high and low values can be made. Prediction models for C8:0, C10:0, C12:0, C14:0, anteiso-C17:0, *c*9-C18:1, MCFA, LCFA, SFA, MUFA and UFA allowed for discrimination between high and low FA values. For these prediction models, the number of L# ranged from five to seven; ideally, a lower number of L# would be preferable. The RER values for models used to predict C8:0, C10:0, C12:0, C14:0, *t*10-C18:1, and C18:3n-3 showed fair practical utility (Williams, 2001).

The relationship between FA concentration and modeling success is shown in Figure 2. Although major individual FA and FA groups (concentration $>$ 5.0 g/kg of milk) presented acceptable r_{CV}, the minor FA and categories exhibited quite variable results. In particular, MCFA and anteiso-C17:0 exhibited r_{CV} similar to those of major FA and categories.

Discussion

FA composition

The FA composition of Brown Swiss milk was consistent with findings from Mele *et al*. (2009) for Holstein Friesian cows reared in north Italy, but it was slightly lower than results reported by DePeters *et al*. (1995) on Brown Swiss milk in a study aimed at comparing the variation of FA composition among three breeds fed and managed similarly in the United States. Regarding the saturation of milk fat, as reported in Table 2, SFA was the most important group of FA followed by MUFA and PUFA; this is in accordance with the literature that reported a normal presence of SFA, MUFA and PUFA of 70%, 25% and 5%, respectively (Grummer, 1991). Regarding the chain length, the MCFA was the most represented group according to Jensen *et al*. (1991). The iso-C14:0, C18:3n-3, *t*10-C18:1, iso-C16:0 and *c*11-C18:1 showed the largest CV (0.47, 0.41, 0.38, 0.37 and 0.37, respectively). The CLA *c*9,*t*11-C18:2 showed lower CV than Mele *et al*. (2009) and Stoop *et al*. (2008).

Prediction models

Prediction models refer to FA concentration in milk (g/kg of milk), which provided better results with respect to prediction models developed for FA concentration in fat (data not shown). This could be explained by a different distribution of values of FA in milk and fat. Moreover, the prediction of FA by MIR is the combined effect of predicting fat content and fat composition and it is performed on milk samples, whereas the reference methods for FA determination (GC) is performed on fat extracted from milk, which means that their relationship is affected by the variation in fat percentage (Soyeurt *et al*., 2006).

On average, the accuracy of the prediction models for major FA was better than for minor FA. This was found also by Soyeurt *et al*. (2006) and Rutten *et al*. (2009), who reported a clear relationship between FA concentration and coefficient of determination (R^2).

Overall, the pre-treated MIR spectra with first derivative or MSC plus first derivative gave the best results; the same mathematical treatments were also the best to predict coagulation properties of milk (De Marchi *et al*., 2009b).

Predictions of FA from our study were slightly less accurate compared with Soyeurt *et al*. (2006) and Rutten *et al*. (2009), probably because of less data availability and low variability of several FA. In particular, the accuracy of prediction models for C10:0, C12:0, C14:0, C16:0 and C18:0 were worse than prediction of the same FA in Soyeurt *et al*. (2006) and Rutten *et al*. (2009); however, similar or better results were found for C8:0, C15:0, *t*11-C18:1, C18:3n-3, *c*9,*t*11-C18:2, *t*9-C18:1 and *c*11-C18:1. Regarding the categories of FA, we detected lower accuracy of prediction models for SFA, MUFA and UFA and similar accuracy for PUFA compared with results from Soyeurt *et al*. (2006). The differences in the accuracy of predictions compared with results reported in literature could be related to several reasons: the variability of the reference data (Rutten *et al*., 2009), the reference method to determine FA composition, the spectra treatments and statistical procedures used to develop the models.

The present study confirmed the potential of MIR for the rapid and non-destructive measurement of several FA. The proposed models are not enough accurate to be transferred to the dairy industry for quality control, but they might become interesting for breeding purposes. Recent studies on milk coagulation properties (Cecchinato *et al*., 2009) and meat physical traits (Cecchinato *et al*., 2011) reported that, despite the accuracy of prediction models being quite low, the genetic response for these traits predicted by MIR was comparable with that obtained using the reference data. Thus, the implementation of models developed in the present study in routine milk recording schemes would allow for selection strategies aiming at improving the FA profile of milk.

Conclusion

The potential of MIR to predict several FA was demonstrated using individual milk samples. The prediction models developed for C8:0, C10:0, C12:0, C14:0, C16:0, anteiso-C17:0, *c*9-C18:1, MCFA, LCFA, SFA, MUFA and UFA were able to identify high and low values of these FA in milk. The methods

using a first derivative or MSC plus first derivative resulted, on average, in the best predictions. Nevertheless, for some FA the improvement in the accuracy was negligible and thus untreated data might be used. However, results evidenced that MIR is not directly applicable to predict detailed milk FA for milk payment system, as suggested by other studies, but the implementation of such models might be evaluated in the future as a tool for breeding programs aimed at enhancing FA content of milk.

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