

Investigation of inter-correlations between fatty acids (FA) and total fat (FAT) in milk and the effect on prediction performance using FT-IR and PLS



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Objectives

Investigate whether individual fatty acids (FA) can be predicted independently of total fat (FAT) using FT-IR and PLS

Conclusions

This study finds that the correlations between FA and FAT cannot be neglected when predicting the FA profile of milk. This fact should be taken into account if building/using calibration models for FA predictions

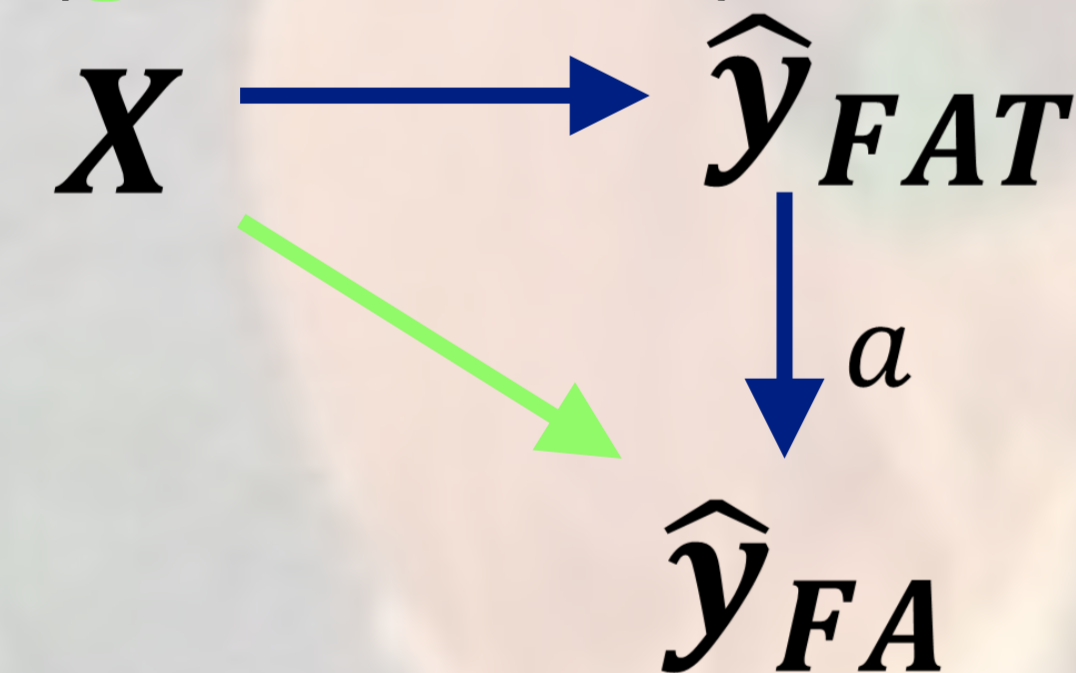
Background

The dairy industry is showing increasing interest in high-throughput methods to predict detailed milk composition including FA profile of milk

SAMPLES: FA were measured with GC in 890 milk samples. Further, FT-IR spectra were recorded for all samples

FAT dependent part and FAT independent part of FA predictions

Predictions of FA in milk can be split into two parts. A FAT related part (**blue arrows**) predicting FAT with a slope correction (a) to match FA. The second part predicts FA independently of FAT (**green arrow**).



Break FA predictions into Sum of Squares (SS)

$$\hat{y}_{FAT} = X \cdot b_{FAT}$$

$$X_0 = (I - \hat{y}_{FAT} \cdot \hat{y}_{FAT}^+) \cdot X$$

$$X_{FAT} = X - X_0$$

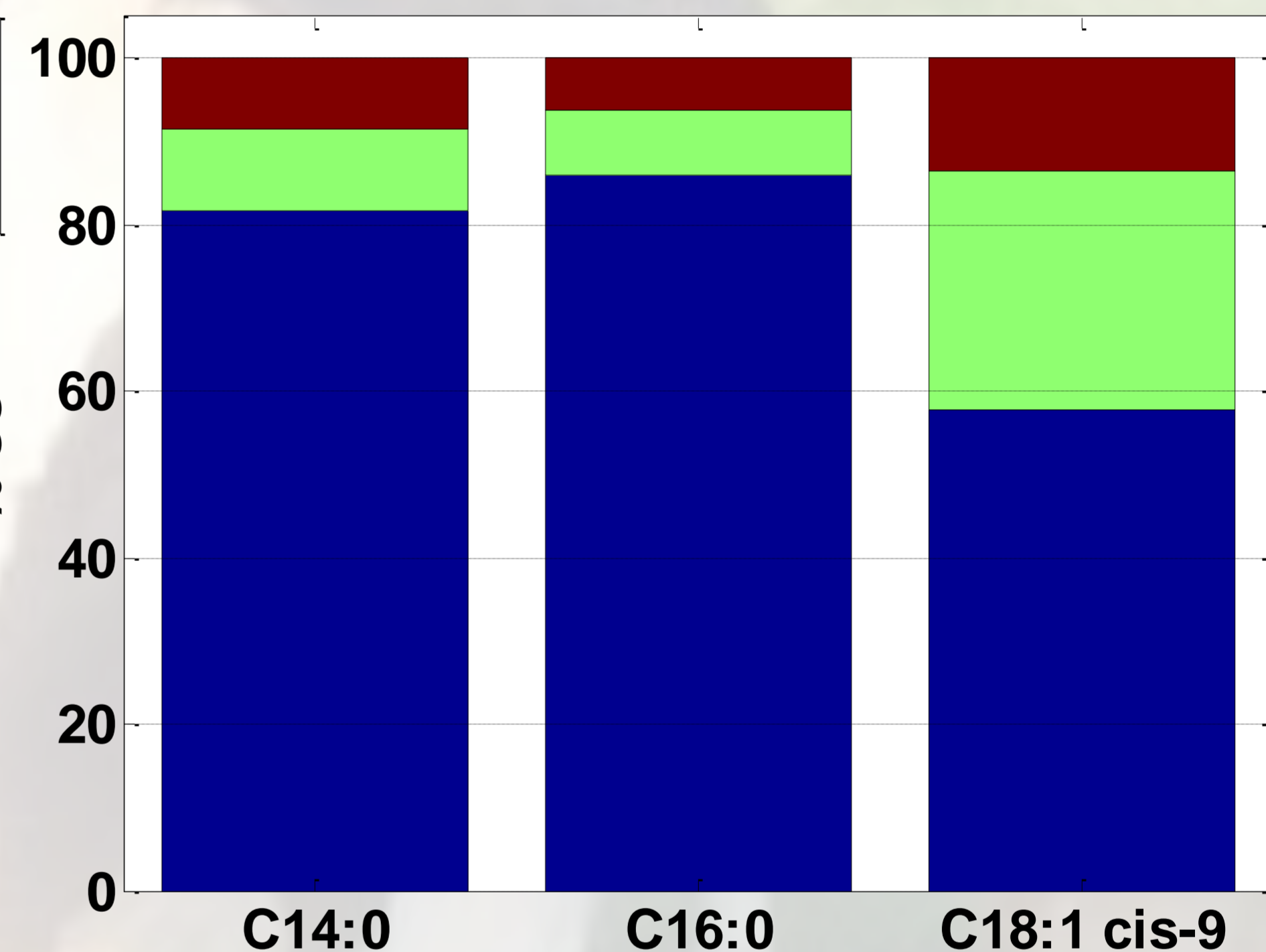
$$y_{FA} = X \cdot b_{FA} + e$$

$$y_{FA} = (X_{FAT} + X_0) \cdot b_{FA} + e$$

$$y_{FA} = X_{FAT} \cdot b_{FA} + X_0 \cdot b_{FA} + e$$

$$SS_{FA} = \underbrace{SS_{X_{FAT} \cdot b_{FA}}}_{\text{FAT related}} + \underbrace{SS_{X_0 \cdot b_{FA}}}_{\text{FAT unrelated}} + \underbrace{SS_e}_{\text{Residuals}}$$

■ Prediction related to FAT
■ Prediction unrelated to FAT
■ Residuals



It is found that FAT has major impact on FA predictions in milk samples

SAMPLES: 17 skimmed milk samples (incl. two replicates) were spiked with FA according to the Simplex Design. FT-IR spectra were recorded for all samples

Predicting FA in Spiked Milk Samples

It is found that FA in milk cannot be predicted independently of inter-correlation relationships (with e.g. FAT) using FT-IR and PLS. Calibration models made to predict FA in milk samples must be used with extra care and it is strictly important that the models are updated to match new samples

