UNIVERSITY OF COPENHAGEN
FACULTY OF SCIENCE

PhD defense

Carl Emil Aae Eskildsen

Prediction of milk quality parameters using vibrational spectroscopy and chemometrics

Opportunities and challenges in milk phenotyping

Time and Location:

May 27th 2016, 1 PM in lecture room A2-70.04, Thorvaldsensvej 40, DK-1871 Frederiksberg C.

The reception will be, after the defense, in room R437, 4th floor (use staircase 6), Thorvaldsensvej 40.

Title
Prediction of milk quality parameters using vibrational spectroscopy and chemometrics - opportunities and challenges in milk phenotyping

Submission
March 11th 2016

Defense
May 27th 2016

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Abstract

Vibrational spectroscopic techniques are widely used throughout all stages of food production. The analysis of raw materials, *real-time* process control, and end-product quality evaluation are all crucial steps in food production. In order to increase production throughput there is a *need for speed* when collecting information from the different processing steps. Hence, conventional methods from analytical chemistry (like Kjeldahl digestion for protein determination) are not compatible with modern production methods.

The aim of this thesis is to show how infrared spectroscopy may and may not be used by dairies and related industries. The focus is specially on possibilities and limitations in applying Fourier transform infrared spectroscopic measurements for detailed milk composition to be used in, for example, breeding programs. Previous studies reported successful predictions of individual fatty acids, protein fractions and coagulation properties from Fourier transform infrared measurements. This thesis shows how such predictions are trapped in a *cage of covariance* with major milk constituents like total fat and protein content. The prediction models for detailed milk composition are not based on causal relationships and this may seriously compromise calibration robustness. It is not recommended to implement indirect models for detailed milk composition in milk recording or breeding programs as such model are providing information on, for example, total protein rather than the specific protein fractions.

If Fourier transform infrared based models on detailed milk composition are to be implemented in, for example, breeding programs it is recommended to decompose, for example, the individual fatty acids into functional groups, such as methyl, methylene, olefinic and carboxylic groups. The average proportions of these groups may be reliable estimated from Fourier transform infrared measurements in contrast to concentrations of individual fatty acids.