Prediction of Enzyme Digestibility of Organic Matter (EDOM) using Spectroscopy and Chemometrics

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[Introduction] Enzyme digestibility of organic matter (EDOM) is an index used in the feed evaluation system for pigs. EDOM is a complex parameter calculated from the protein, carbohydrate, starch and fiber fractions in the forage and it is therefore a challenge to relate EDOM to specific chemical bounds. The aim of this project is to investigate the possibility of using near infrared (NIR) reflectance spectroscopy to predict EDOM in wheat and triticale and to investigate if it is possible to develop a global NIR model on wheat and triticale.

[Materials and Methods] Reflectance spectra of 153 dried and ground wheat and triticale samples were obtained using a QFA-Flex 400 FT-NIR instrument (Q-interline, Roskilde, Denmark). The samples were packed in glass vials with a height of 6 cm and a diameter of 2.6 cm and measured using a rotating sample device. The sample was rotated with a speed of three rounds per minute, with a measuring sample window at the rotating sample device has a diameter of 6 mm and the analysis surface is $\sim 510 \text{ mm}^2$. NIR measurements in the range from 4004 to 9088 cm⁻¹ with data collection at every 5 cm⁻¹ were performed on grounded and dried aliquots. The spectra are reported as log (1/*R*). Principal component analysis (PCA) and partial least squares regression (PLSR) were preformed. The global (wheat and triticale samples) and local (wheat or triticale samples) calibration models were validated using segmented cross validation with 10 segments. Afterwards the global calibration model was validated using an independent test set of 51 samples. The local models on each species were validated using the other specie as test set. In this way the ability of the models to be extrapolated to different species was tested. Outlier detection was based on PCA, Tvs.U and influence plots.

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[Results and Discussion] The global PLSR validated model used 8 PLSR principal components, has a correlation (R) of 0.80 and an RMSECV of 0.49 EDOM. The loading plot of the 3 first loadings shows that several of them contain information. Especially in the wavelength area of 4500, 5400 and 7300 cm⁻¹ there is much information. The conclusion is that prediction of EDOM using NIR reflectance spectroscopy has a lower prediction error than the error allowed between duplicate wet chemical measurements (2%). It is possible to predict EDOM by ± 1.24 EDOM in a range from 89.8 to 93.5 EDOM. To evaluate this error it is necessary with a more realistic calculation of error from the wet chemical method. In the present project only one duplicate measurement of EDOM was available and several more repeated measurements are necessary in order to calculate the reproducibility of the wet chemical method. If the purpose is to use the NIR model in a screening process the present error is probably acceptable.

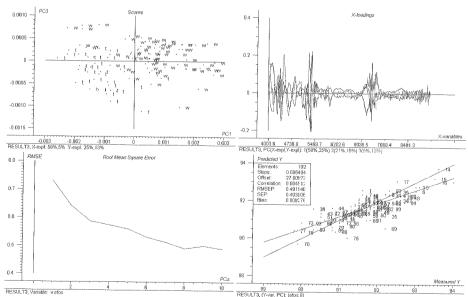


Figure 1. Final global PLSR model on 1d and MSC pre-processed NIR spectra.

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