Prediction of enzyme digestibility of organic matter (EDOM) using spectroscopy and chemometrics

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Introduction

Wheat and triticale are a primary energy source in the feedstuffs in swine diets. Enzyme digestibility of organic matter (EDOM) is an index used in the feed evaluation system for pigs. This is based on the close linear relationship between the in-vitro enzyme digestibility of organic matter and in -vivo total tract digestibility of energy.[1] EDOM is a complex parameter calculated from the protein, carbohydrate, starch and fibre fractions undergoing a three-step enzymatic incubation. It is therefore a challenge to relate EDOM to specific chemical bonds.

Near infrared reflectance (NIR) spectroscopy has become a widely used method in analysis of a range of agricultural products, due to its rapidness and low maintenance cost, and has been extensively reviewed.[2,3] NIR spectroscopy is therefore a very interesting tool for animal feed control.

The aim of this study was to investigate the possibility of using NIR spectroscopy to predict EDOM in wheat and triticale, and to investigate the possibility of developing a global NIR model for wheat and triticale.

Materials and methods

Samples of wheat and triticale varieties (153) with known in-vitro and in-vivo digestibility values were used (Table 1).

Table 1. Total number of samples (*n*), mean, range and standard deviation (*SD*) of EDOM in all samples and within species.

	N	Mean (EDOM)	Range (EDOM)	SD (EDOM)
All samples	153	91.6	89.8–94.0	0.8
Wheat (w)	103	91.8	90.0–94.0	0.8
Triticale (t)	50	91.0	89.8–92.7	0.7

The *in-vitro* ileal and faecal digestibility methods used have been described in earlier publications.[1,4]

Reflectance spectra of the 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 samples were rotated at a speed of three rounds per minute with a measuring sample window at the rotating sample device. The window has a diameter of 6 mm and the analysis surface is ~ 510 mm^2. NIR measurements in the range from 4004 to 9088 cm^{-1} with data collection at every 5 cm^{-1} were performed on ground and dried aliquots. The spectra are reported as log (1/*R*). Principal component analysis (PCA) and partial least squares regression (PLSR) were performed. The global (wheat and triticale samples) and individual (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 individual models of each species were validated using the other species 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, X-Y relation outlier plots and influence plots.

Results and discussion

Table 2 shows the calibration and test set.

The "sorted" calibration set consists of wheat and triticale and was validated using the "sorted" test set which also consisted of both wheat and triticale. The wheat calibration set was only validated using wheat samples in the test set and same procedure was used for the triticale data set. The global PLSR validated model used 8 PLSR principal components, giving a correlation coefficient (*R*) of 0.80 and an *RMSECV* of 0.49 EDOM (Table 2). The table includes total the number of samples used in the calibration or validation set (n), number of partial least squares regression components (#PLSR), regression coefficient (*R*), root mean square error of cross-validation (*RMSECV*), root mean square error of prediction (*RMSEP*), standard error of prediction (*SEP*) and bias. Results are shown for pre-processed (1d, MSC) NIR spectra. The loading plot of the 3 first loadings shows that several loadings contain much information, particularly in the wavelength area of 4500, 5400 and 7300 cm^{-1}. 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 units in a range from 89.8 to 93.5 EDOM. To evaluate this error it is necessary to determine a more realistic calculation of the error of 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 considered to be acceptable.

It is not surprising that prediction of EDOM using NIR spectroscopy is not very effective. Compared to prediction of e.g. protein using NIR spectroscopy, EDOM is a much more complex parameter to predict, because it is an index of several parameters. This is evident from the loading plots, where several wavelength areas contribute information. It is therefore also logical that the number of latent variables needed to predict EDOM would be higher, compared to prediction of protein content.

Table 2. Calibration and validation statistics of PLSR models on NIR spectra (4004 cm^{-1} to 9088 cm^{-1}) for determination of EDOM in wheat and triticale.

Calibration						Test set						
Samples	*n*	Range (EDOM)	#PLSR comp.	*R*	*RMSECV* (EDOM)	Samples	*n*	Range (EDOM)	*R*	*RMSEP* (EDOM)	*SEP*	Bias
Sorted	100	89.8–94.0	8	0.80	0.49	Sorted	51	89.8–93.5	0.66	0.62	0.62	0.03
Wheat	101	90.0–94.0	9	0.74	0.52	Triticale	50	89.8–92.7	0.64	0.53	0.54	0.03
Triticale	48	89.8–92.7	4	0.65	0.50	Wheat	103	90.0–94.0	0.40	1.57	0.87	1.31

References

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