Prediction of the nutritional composition of dried distiller's grains and solubles by NIRS

Objective:
Evaluate the feasibility of making NIRS calibrations for amino acids and energy for dried distiller's grains and solubles (DDGS).

Materials and methods:
A total of 103 samples of DDGS were obtained from Dr. Jerry Shurson, University of Minnesota. These samples were obtained from 9 different plants over a period of two years and had been analyzed upon receipt for amino acids by the University of Missouri using AOAC approved methodology. At the request of Dr. Joe Hahn, Hubbard Milling, Mankato, MN, retained subsamples were shipped to Dr. Theo van Kempen, North Carolina State University for analysis by NIRS.

Upon receipt of the samples in North Carolina, samples were ground using a Retsch grinder through a 0.5 mm screen. Aliquots were analyzed for gross energy using an IKA model C5000 bomb calorimeter (analysis performed in duplicate). Ground samples were analyzed using a NIR Systems model 6500 spectrophotometer using a half-size rectangular cup. Scans were obtained from 400 to 2500 nm. Spectral data were derivatized to the 2nd order and smoothed, and calibrations were developed using partial least squares regression with cross-validation (20 segments) using The Unscrambler after removal of outliers.

Results:
For Lys, Met, Thr, and energy, calibrations were developed using PLS1 (Table 1). With this method, calibrations are developed for individual parameters. The calibrations obtained were only reasonable, with over 75% of the variation explained for Lys and energy, and 53 and 66% of the variation for Thr and Met, respectively. For Thr, the reason for disappointing calibrations is likely the low variation within the samples, with a CV of only 6.2%. For Met, a better calibration was expected especially given the large variation and the fact that calibrations for Met in feedstuffs such as meat and bone meal are very successful. For energy, a reasonable calibration was developed especially given the low variation in energy content between the samples (CV of 1.9%).

Table 1. Calibration statistics obtained using PLS1. R is the correlation between actual and predicted values, and rmsep is the prediction error.

	R	Rmsep, %	R^2	CV, %
Lys	0.89	0.064	0.79	16.2
Met	0.81	0.044	0.66	14.2
Thr	0.73	0.046	0.53	6.2
Energy	0.87	37	0.76	1.9

The data were also used to make a PLS2-type calibration (Table 2). With this type of calibration, multiple dependent variables are calibrated for at the same time, in this case, all the amino acids. Arguments for using PLS2 is that it is a faster method of calibrating, but more importantly, the calibration developed can take the interdependence of the variables in consideration, thus resulting in calibrations that are more biologically relevant/robust. A disadvantage of PLS2 is that the calibration is not optimized for individual parameters as outliers for a specific parameter are not removed. For amino acids, this may be especially important as three different assays are used. The calibration results indeed show that the calibration obtained with PLS1 is better than the calibration obtained with PLS2. This difference was large for Lys and Thr and minimal for Met.

Table 1. Calibration statistics obtained using PLS2. R is the correlation between actual and predicted values, and rmsep is the prediction error.

	R	Rmsep, %	R^2	CV, %
Thr	0.61	0.050	0.37	6.2
Cys	0.74	0.035	0.55	9.4
Val	0.65	0.078	0.43	7.3
Met	0.80	0.046	0.64	14.2
Ile	0.71	0.065	0.50	8.5
Leu	0.84	0.125	0.70	6.5
Phe	0.82	0.052	0.68	6.5
His	0.76	0.036	0.58	7.8
Lys	0.73	0.089	0.53	16.2
Arg	0.75	0.065	0.56	8.7
Trp	0.60	0.017	0.36	9.1
TAA	0.79	1.008	0.63	6.6

Conclusion:

Calibrations for amino acids and energy in dried distiller's grain and solubles can be developed using NIRS. The quality of these calibrations is dependent on the calibration method used, with PLS1 calibrations preferred over PLS2 calibrations. Overall, the quality of these calibrations was only reasonable, especially compared to the quality of calibrations that can be developed for feedstuffs such as meat and bone meal which is also a very heterogeneous and heat processed material. From this study it is difficult to determine the reason for this. Possibilities include 1) assay variation over time for the DDGS. 2) The generally lower amino acid concentrations in DDGS compared to MBM. 3) The small samples analyzed by NIRS were not representative of those assayed for amino acids.