# Technological evaluation of groat percentage in oat (*Avena sativa* L.) genotypes by near infrared spectroscopic analysis

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## Introduction

A very serious constraint in the use of oat (*Avena sativa* L.) cultivars is the presence of hulls on the kernel. The hulls (lemma and palea) are leaf-like structures that tightly enclose the groat and provide protection for it. During early development, the hulls contain photosynthetic and vascular tissues, which contribute largely to groat nutrition. At maturity, however, they are dry, brittle and devoid of any significant metabolic activity.[1] The hulls are important in keeping the groat clean and free from moulds and other fungi. Groats that protrude from the lemma and palea at maturity, in the presence of sufficient moisture, may become infected with pathogens.[2]

The hulls have a low protein content, about 1–2% of the total kernel protein,[1] but are high in total dietary fibre (about 80% according to Marlett[3]) and, therefore, are not easily digested by non-ruminants. Burrows[4] considered that the high fibre content of hulls lowers the intrinsic energy of the grain for feeding purposes; Forsberg and Reeves,[2] on the other hand, considered the hulls valuable as roughage in animal feed.

The hulls contribute to total kernel weight by 20% to 30%.[1] Cultivars show a large variation in the percentage of hulls, which is even greater when environmental conditions affect the extent to which the groat is filled.[4] Pomeranz *et al*.[5] reported that small kernels had a small hull content (26.8%), whereas coarse kernels have a high hull content (33.4%).

Groat-to-hull ratio is a reliable and widely used indicator of oat grain quality. Several workers reported that the groat fraction was superior to test weight as an indicator of the whole grain quality.[6,7] For a long time, mechanisms to evaluate seed samples quickly, efficiently and accurately for groat-to-hull ratios has not been available.[2] In our laboratory, groat percentage is evaluated gravimetrically, quantifying the percentages of groats and hulls obtained from a sample of 50 g after one pass in a de-hulling apparatus. This procedure is quite slow and time-consuming, as it is necessary to determine the exact weight of the sample before de-hulling and of the two fractions recovered. Moreover, it is subjected to experimental errors.

Near infrared (NIR) reflectance spectroscopy analysis is a consolidated method to evaluate chemical characteristics of the cereal caryopses, such the content of protein, carbohydrates, fat, water, fibre and so on.[8–12]

The aim of this study was to develop NIR reflectance spectroscopy calibration equations for groat percentage in oats, in order to characterise the genotypes currently grown in Italy.

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## Materials and methods

### Plant material

The oat genotypes considered in this study were grown, in replicate, during the years 1996–1998, in several environments across Italy.

### Sample preparation

A sample of about 200 g from each replication was collected for all the genotypes. In 1996 and 1997, 50 g of each sample were mechanically de-hulled, using a Irom Otake instrument. The amount of de-hulled seeds, expressed as a percentage of the weight of the sample, was registered as "groat percentage". Both intact and de-hulled kernels (here defined as "grain" and "groat", respectively), were milled using a Cyclotec Udy Mill with a 1 mm sieve and submitted to NIR reflectance spectroscopic analysis. A set of samples harvested in 1997 ($n$ = 129) and all the samples harvested in 1998 were collected and submitted to NIR reflectance spectroscopic analysis without the de-hulling and milling steps.

### NIR reflectance spectroscopy analysis

Approximately 2 g of each ground sample, or 20 g of each intact sample, were packed into a black aluminium sample cup containing a rectangular quartz window. Samples were irradiated with near infrared monochromatic light and the diffuse reflectance collected by means of lead sulphide detectors in a Foss NIRSystems 6500 scanning monochromator. All spectral data were recorded as log 1/$R$ where $R$ = reflectance, in the wavelength range 1100–2498 nm, at every 2 nm, to give a total of 700 data points per sample. The mathematical transformation (1, 5, 5) of the spectral data was carried out before derivation of the regression models. The first number indicates the derivative used, the second is the length of the segment expressed as data points and the last shows the length of the smoothing segment. A modified partial least squared (MPLS) regression technique was used to develop the calibration equations. The equation selected as the best for each chemical fraction was obtained using the following criteria:

1. The lowest standard error of cross-validation; this was obtained by dividing the data into sets of four and predicting each fourth value by calibrations developed from the other three values. Samples with large residuals were omitted and cross validation was performed again.
2. The wavelengths that correspond most closely with the particular chemical fraction.
3. Test of predictive performance by applying it to the remaining validation samples and calculating the standard error of prediction (*SEP*) and the variance accounted for ($R^2$ validation), in line with the procedures described by Windham *et al.*[13]

Predicted values were related to corresponding laboratory analyses by simple linear regression. *SEP,* $R^2$, slope and difference between laboratory analysis and prediction means were used to test whether an equation had successfully predicted the values of the validation set.

## Results

NIR reflectance spectra were collected from intact and ground samples of 15 genotypes grown in 1996, 1997 and 1998. In 1996, the number of samples considered was 400; they were analysed, both as grains and groats, giving a total of 800 NIR reflectance spectra. A subset of 94 samples for each group were then chosen for calibration. In 1997, 480 samples were analysed, giving a total of 960 NIR reflectance spectra. The samples used for calibration were 103 for groats and 187 for grains. In the same year, a set of 129 samples were arbitrarily chosen among the replications, analysed by NIR reflectance spectroscopy as intact grains and then de-hulled. The values of groat percentage obtained were used for calibration. Finally, in 1998, a set of 191 samples (intact grains) were collected and were

**Table 1. NIR reflectance spectroscopy statistical parameters for groat percentage in the samples collected in 1996,1997 and 1998.**

| Material | Year | Number of samples[a] | Mean | *SEC* (%)[b] | $R^2$ | *SECV* (%)[b] | 1–*RV* |
|---|---|---|---|---|---|---|---|
| Groats (ground) | 1997 | 103 | 68.6 | 2.58 (3.8%) | 0.61 | 2.97 (4.3%) | 0.50 |
| Grains (ground) | 1997 | 187 | 68.6 | 2.77 (4.0%) | 0.68 | 3.08 (4.5%) | 0.61 |
| Grains (intact) | 1998 | 106 | 69.3 | 2.24 (3.2%) | 0.64 | 2.54 (3.7%) | 0.55 |

*SEC* = standard error of calibration; $R^2$ = multiple regression coefficient; *SECV* = standard error of cross-validation
1–*RV* = regression coefficient for cross-validation
[a] Number of samples used for calibration
[b] Percentage of the mean value

used for calibrations. Finally, in 1998, a set of 191 samples (intact grains) were collected and analysed by NIR reflectance spectroscopy; two spectra were recorded for each sample. Groat percentage was evaluated by de-hulling; the value obtained was the mean of two replicates. A subset of 106 spectra were then chosen for calibration. Table 1 shows the statistical parameters related to the best calibration equations obtained for each type of material analysed.

For ground groats the best equation was obtained with genotypes grown in 1997. The correlation coefficient ($R^2$ = 0.61) was lower than the one we obtained in a previous calibration, but was related to a dramatic reduction of both *SEC* and *SECV* values (–32% and –47%, respectively), compared with the first equation.

Groat percentages for ground grains (1997) showed an $R^2$ value of 0.68. In this case, too, the standard error was found to be lower than in the previous equation: *SEC* and *SECV* decreased from 4.1% and 5.0%, respectively, (data not shown) to 4.0% and 4.5% (Table 1) in this equation.

A calibration equation was developed, also using intact grains: it was characterised by a quite interesting $R^2$ value (= 0.64) and by the lowest error for calibration and cross-validation, 3.2% and 3.7%, respectively (Table 1).

## Discussion

The importance of groat percentage in the characterisation of oat genotypes is principally bound to their use in the food or pharmaceutical industries, as, in these applications, the raw material must necessarily be de-hulled. So far, a quick and reliable method to determine groat percentage in small samples of seed has been lacking. It must be considered, also, that mechanical de-hulling is a time-consuming procedure and it is subjected to experimental error.

In this study we propose the application of NIR reflectance spectroscopy to predict groat percentage in oat genotypes. Calibration equations were developed, both in intact and ground grains. The results indicate that a correlation can be drawn between the groat percentage of a sample and its NIR reflectance spectrum and the value of the correlation coefficient was quite interesting. Both grains and groats can be used for this analysis, with good results and acceptable levels of *SEC* and *SECV*. More interesting is the possibility of analysing intact grains directly, which eliminates the necessity to de-hull and/or mill the samples. The correlation coefficients of the equations developed for intact grains are lower than the ones obtained with the ground material, but the advantages are many.

NIR reflectance spectroscopic analysis can, therefore, be considered a suitable and effective technique to predict groat percentage in oat genotypes. The possibility of applying this technique to predict the hull percentage and/or the milling yield of other cereals should also be considered.

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