Comparison of near infrared transmittance and near infrared reflectance spectroscopy to select high nutritional value naked oats

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Introduction

Oats (*Avena sativa*) are unique among cereals, being a rich source of soluble fibre (β-glucan), good nutritional value proteins, vitamins and natural specific antioxidants. In addition, oats contain high amounts of unsaturated lipids. Therefore, the interest in oats for the production of functional foods is increasing, due to both their nutritional quality and the indication of health benefits related to oat consumption. The growing evidence of the physiological effects and the positive impact of soluble fibre on some of the risk factors of cardiovascular diseases[1,2] have stimulated a great interest in oats, particularly for their high β-glucan content. β-Glucan is a large, linear non starch polysaccharide (β(1→3)/(1→4)-D-glucose units) mainly localised in the endosperm cell wall of oat and barley,[3] and able to produce highly viscous solutions.[4] This characteristic is linked with its potential health benefits.[5] Because of this, β–glucan is predicted to become an important component in human nutrition. As a consequence, raw material more suitable for oat-based food production is in demand. To achieve this aim, breeding programs for naked oat (more suitable than hulled oat for food production) improvement[6] need fast and accurate methods for β–glucan determination during the selection of high quality lines. The traditional analytical methods for β–glucan quantification[7–9] require long determination times, high costs and are destructive of the sample. Near Infrared Spectroscopy could be suitable for this purpose in relation to its well-known advantages.[10]

Concerning the cereal fibre components, previous works have shown the ability of NIR reflectance and NIR transmittance technology to quantify soluble and insoluble dietary fibre in kernels.[11] Other authors have demonstrated the possibility of using NIR reflectance spectroscopy to analyse barley for β–glucan content.[12–15] Recently, Schmidt *et al.*[3] compared the ability of different kinds of NIR instruments to measure β–glucan content in naked barley.

The aim of the present study was to investigate the possibility of determination of β–glucan content simultaneously with other quality parameters of naked oat, by using near infrared spectroscopy. The performance of transmission *vs* reflectance instruments, as well as the effect of sample treatment (whole kernels and milled groats) were also evaluated.

Materials and methods

The data set comprised naked oat samples, from 12 different varieties, harvested in Italy and other European countries in the years 2006–2009. An aliquot of each sample was milled to a particle size of 0.5 mm using a Fritsch 14.702 mill. Transmission measurements (grain and flour) were recorded on a grain analyser (Infratec 1241, FossItalia, Pd) in the wavelength range of 800–1048 nm at 2 nm intervals (Figure 1).

Pathlength was 18 mm (whole grain) or 3 mm (flour). Reflectance spectra were collected using a Foss NIR-system model 6500, equipped with a sample transport module (wavelength range 400–2498 nm) scanning at 2 nm intervals (Figure 2).

Protein content was assessed by the Kjeldahl method. β-glucan concentration was measured according to the enzymatic method of Mc Cleary and Codd[7] using Megazyme β-glucan kit. In all cases the spectra collected were pretreated (detrending, SNV and 1st derivative) and calibration models built using PLS regression.[16]

Results

Calibration

Protein and β-glucan contents were analysed in naked oat samples and the results were used for model development and external validation. 5-fold cross-validation was used to determine

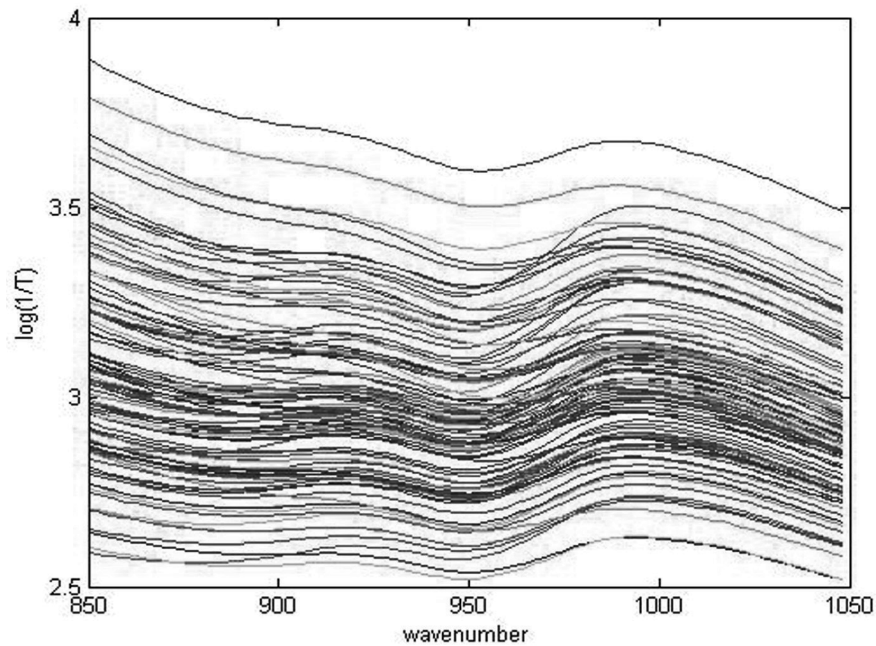

Figure 1. Example of NIR transmittance spectra (milled oat) of samples used for calibration.

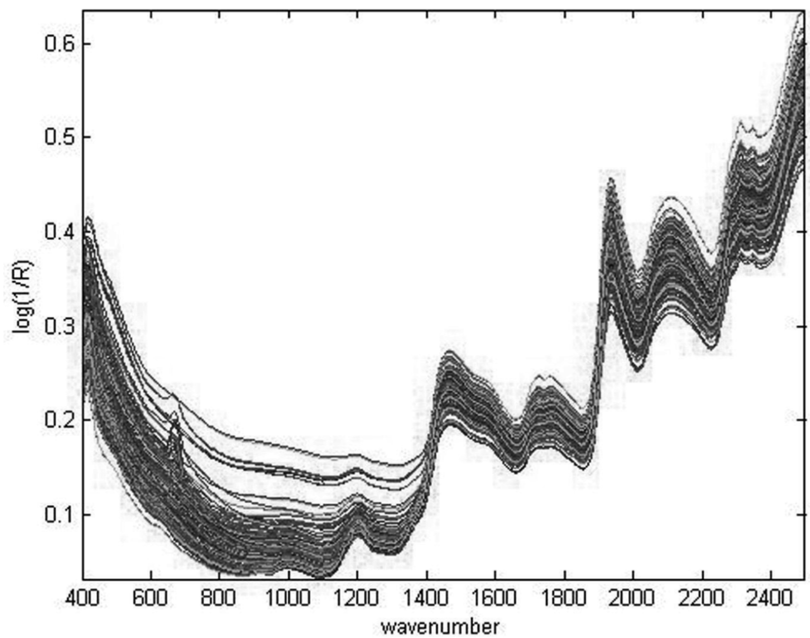

Figure 2. Examples of NIR reflectance spectra (milled oat) of samples used for calibration.

the optimal complexity in the model development phase. Calibration results are summarised in Table 1.

The three data sets had a different numbers of samples, and exhibited a large protein content range (% as is), but a more limited β-glucan content range (% as is). The resulting models showed high R^2 values for protein prediction. The best calibration equation developed for β-glucan resulted in an R^2 value of 0.73 (NIR reflectance on milled grain). In general, the performances of NIR transmittance whole grain models were slightly poorer than those based on milled grains, as previously shown[17].

NIR transmittance whole grain validation

External validation was carried out on an additional set of 16 measurements ranging from 13.2 to 17.5 and from 3.0 to 3.7 for protein and β-glucan contents, respectively. The *SEP*s obtained were 0.576 and 0.211 for protein and β-glucan, respectively. These results confirmed that the NIR transmittance models developed for determining these quality parameters in whole grain produced results with an accuracy adequate for fast quality evaluation of naked oat lots, at least for protein content. Moreover, the use of whole grains could meet the requirements to process the raw material non-destructively.

NIR reflectance and transmittance milled grain quality control

The suitability and accuracy of the NIR transmittance and NIR reflectance models developed on milled grain data sets, was evaluated on a group of naked oat breeding lines. The results of the

Table 1. Statistical summary and calibration results for PLS modelling of naked oat qualitative parameters.

Parameters		Raw materials	*n*	Mean values	Min.	Max.	St. Dev.	R^2	*SEC*	*SECV*
Protein	NIR transmittance	Whole Grain	185	16.22	12.48	20.01	1.67	0.942	0.380	0.400
		Milled Grain	94	15.74	12.93	19.62	1.67	0.970	0.268	0.278
	NIR reflectance	Milled Grain	320	16.30	12.48	21.53	1.69	0.968	0.280	0.302
β-glucan	NIR transmittance	Whole Grain	183	3.37	2.24	4.17	0.37	0.549	0.233	0.238
		Milled Grain	92	3.19	2.01	4.17	0.47	0.674	0.265	0.269
	NIR reflectance	Milled Grain	304	3.41	2.39	4.33	0.35	0.731	0.164	0.180

Table 2. Comparison of NIR transmittance and NIR reflectance performance for quality evaluation of ten naked oat breeding lines (milled grain). Protein content: mean value: 15.00, range: 13.09–16.53; β-glucan content: mean value 3.40, range: 3.16–3.66.

Naked oat breeding lines	Protein		β–glucan	
	Residual			
	LAB vs NIR reflectance	LAB vs NIR transmittance	LAB vs NIR reflectance	LAB vs NIR transmittance
1	0.226	0.312	0.087	0.015
2	0.303	0.028	0.006	0.128
3	0.116	0.568	0.060	0.191
4	0.282	0.302	0.013	0.329
5	0.419	0.246	0.094	0.121
6	0.518	0.381	0.023	0.080
7	0.136	0.173	0.280	0.149
8	0.050	0.378	0.373	0.053
9	0.368	0.372	0.511	0.483
10	0.178	0.003	0.298	0.346
Mean	0.260	0.276	0.175	0.190
Min	0.050	0.003	0.006	0.015
Max	0.518	0.568	0.511	0.483
St. Dev.	0.147	0.172	0.178	0.150
SEP	0.165	0.173	0.192	0.242

quality control of advanced breeding lines are presented in Table 2 as residuals between reference (LAB data) and NIR transmittance or NIR reflectance predictions.

In this table the *SEP* values of validation are also reported. The low residuals and *SEP* values indicate the good performance of the calibrations for rough selection of large populations of naked oat breeding lines. In fact, the results obtained in the validation tests showed good prediction ability both of NIR transmittance and NIR reflectance models, the data being comparable with reference values.

Conclusions

The simultaneous measurements of protein and β-glucan contents in naked oat grains could be carried out by coupling NIR transmittance and NIR reflectance and chemometrics, with the accuracy required for screening samples, and with significant advantages to reduce costs and speed up specific quality breeding programs. In milled samples NIR spectroscopy showed better performance than NIR transmittance technology, probably because the limited wavelength range provided less information. The results obtained in this work for β-glucan prediction were in accordance with the findings of Schmidt *et al*.[3] in naked barley by using analogous instruments. Although the possible range of β-glucan content for our breeding lines was limited, reasonable accuracy in both internal and external validation was observed. On the basis of the present results, additional tests with a calibration data set containing a wider range of composition should allow the establishment of a more robust β-glucan prediction model, valid for different naked oat cultivars.

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