Near infrared reflectance spectroscopy for quality evaluation of *Triticum monococcum*

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Introduction

Einkorn (*Triticum monococcum* ssp *monococcum*), a diploid hulled wheat carrying the A genome (2n = 2x = 14), was among the crops that founded agriculture in the Near East.

In recent years interest in the qualitative aspects of primitive wheat has grown, in view of the development of new or special foods. Because of its characteristics, einkorn appears to be a promising candidate for the production of cookies or bread with high protein content and bright yellow colour and has been recently reconsidered as potentially interesting for future cultivation.[1]

The high level of variability for several traits affecting yield and resistance makes einkorn suitable for a breeding programme aimed at selecting superior lines. In this context there is a need to develop rapid and accurate screening methods for quality trait evaluation.

The aim of this work was to develop NIR calibrations for chemical composition and rheological parameters of einkorn whole meal and flour.

Materials and methods

The einkorn samples considered were grown in replicated plot trials in two locations (Milan and Cologne) in1995 and 1996. Seeds from the three replications of each trial were blended and a sample of about 2 kg per line was dehulled with an Otake FC4S apparatus (Satake, Japan). A sub-sample of dehulled grain (30 g) was ground with a 1 mm sieve Cyclotec mill (Tecator, Sweden). The remaining grain was tempered overnight at 15% moisture and milled with a Bona 4RB (BONA, Italy) experimental mill.

Hardness, moisture, protein content (N × 5.7), SDS sedimentation volume, dry gluten, farinograph and cookie test were performed according to the procedures listed in Table 1.

NIR analysis was performed with an Infraalyzer 500 monochromator (Bran+Luebbe, Germany).

For each sample NIR spectra in apparent absorbance (Log 1/*R*) at intervals between 1100 and 2500 nm, with a step of 4 nm, were collected in duplicate, then averaged and recorded as one spectrum per sample. Samples were divided into calibration and validation sets with the same range of variation for each constituent.

Calibrations based on multiple linear regression (MLR) were performed by the "Step-up search" programme (Idas-System-Bran+Luebbe software).

For dry gluten, farinograph and cookie indices, calibrations were also performed by partial least square (PLS) regression (Sesame, Bran+Luebbe software).

Table 1. Laboratory procedures.

Parameter	Method
Hardness	AACC 39-70A (1997)
Moisture	AACC 44-19 (1995)
Protein content	DUMAS modified (Kirsten, 1983)
SDS sedimentation volume	Preston et al. (1982)
Dry gluten	Glutomatic apparatus
Farinograph	ICC 115-D (1972)
Cookie quality	AACC 10-52 (1995)

Calibration performances were evaluated as correlation coefficient (*r*), standard error of estimate (*SEE*), standard error of prediction (*SEP*) and ratio of standard error of prediction to standard deviation (RPD) calculated by dividing the standard deviation of the reference values by the *SEP*.[2]

Results and discussion

Whole meal

All the samples presented a very soft texture as determined by NIR on whole meal. The hardness indexes ranged from 6 to 24 (data not reported) with a mean value of 16, remarkably lower than 40, considered as the threshold for soft wheat.[3] In Figure 1 the spectrum of the *T. monococcum* whole meal sample with the highest hardness index (24) is reported along with the spectra of two *T. aestivum* whole meal samples with hardness index of 40 (soft wheat) and 92 (hard wheat), respectively.

The range, mean and standard deviation values for moisture, protein content and SDS sedimentation volume of einkorn whole meal are reported in Table 2. The variability in SDS sedimentation volume among einkorn lines was largely independent from protein content but was significantly correlated with bread volume.

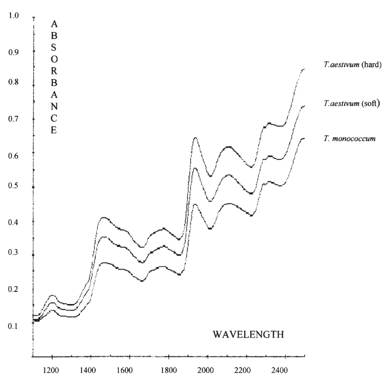

Figure 1. Comparison among spectra of the einkorn whole meal with the highest hardness index and of two wheat whole meals.

The NIR calibration statistics for each constituent are reported in Table 3 and in Figures 2 (a) and (b). Good correlations were obtained for moisture (*r* = 0.99; *SEP* = 0.11) and protein content (*r* = 0.98; *SEP* = 0.30), while for SDS sedimentation volume the results appeared inadequate (*r* = 0.78; *SEP* = 6.24). For this parameter the low RPD value (2.2) indicated that the variation due to the NIR model is almost the same as the naturally occurring variation: thus, the provisional ability of NIR model seems to be low and only useful for breeding purposes.

Flour

The range, mean and standard deviation values of the flour constituents considered are reported in Table 4. A high degree of variability

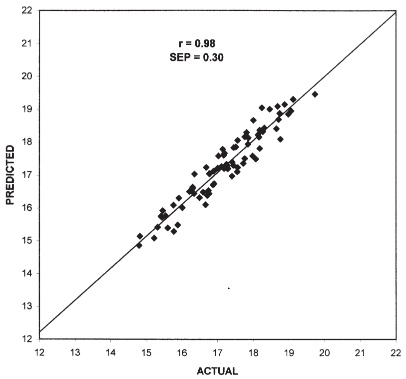

Figure 2(a). NIR v. analytical data of the validation set for protein content in whole meal.

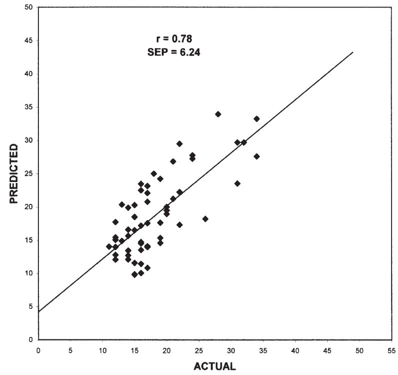

Figure 2(b). NIR v. analytical data of the validation set for SDS sedimentation volume in whole meal.

was detected for protein content, SDS sedimentation volume and dry gluten. Farinograph water absorption ranged from 52.6 to 61.4% and stability from 24 to 450 sec. Doughs were often sticky: gluten and readable farinograms have been obtained only on a reduced number of samples.

The calibration models were good for moisture and protein content and satisfactory, but only for breeding purposes, for SDS sedimentation volume (Table 5). None of the remaining parameters seemed to be accurately predicted by NIR.

In the case of water absorption the results obtained are in contrast with those reported for wheat flour:[4,5] This is probably due to the different composition in starch granules of the two species. Einkorn infact, as compared to wheat, presents a high percentage of small starch granules (type B) that could affect the water absorption index without any relation with protein content and composition.[6]

Table 2. Mean, standard deviation (SD) and range of analytical values for calibration sets of einkorn whole meal.

Parameter	N samples	Mean ± SD	Range
Moisture (%)	74	13.6 ± 1.7	10.6 – 14.7
Protein content (%)	59	17.6 ± 1.5	15.2 – 21.9
SDS sedimentationvolume (mL)	68	32 ± 14	11 – 51

Table 3. Statistics for calibration (*r*, *SEE*) and validation (*SEP*, RPD) of einkorn whole meal.

Parameter	*r*	*SEE*	*SEP*	*RPD*[a]
Moisture (%)	0.99	0.08	0.11	15.5
Protein content (%)	0.98	0.30	0.34	4.4
SDS sedimentation volume (mL)	0.78	6.24	6.42	2.2

[a]*RPD* = standard deviation of biochemical value * SEP^{-1}

Table 4. Mean, standard deviation (SD) and range of analytical values for calibration sets of einkorn flour.

Parameter [(a)]	N. samples	Mean ± SD	Range
Moisture (%)	42	14.4 ± 1.7	9.4 – 16.7
Protein content (%)	77	16.6 ± 1.4	12.8 – 19.9
SDS SED VOL (mL)	120	38 ± 27	7 – 98
Dry gluten (%)	49	7.9 ± 6.7	0.1 – 17.1
FAR WAT ABS (%)	50	55.9 ± 2.2	52.6 – 61.4
FAR STAB (sec)	49	119 ± 108	24 – 450
Cookies width (cm)	40	9.29 ± 0.42	8.43 – 10.03
Cookies height (cm)	40	0.70 ± 0.06	0.59 – 0.80

[a]SDS SED VOL = SDS Sedimentation volume
FAR WAT ABS = Farinograph water absorption
FAR STAB = Farinograph stability

Table 5. Statistics for calibration (*r*, *SEE*) and validation (*SEP*, RPD) of einkorn flour.

Parameter	*r*	*SEE*	*SEP*	RPD
Moisture (%)	0.98	0.09	0.12	14.2
Protein Content (%)	0.97	0.28	0.28	5.0
SDS SED VOL (mL)	0.83	15	13	2.1
Dry gluten (%)	0.79	4.4	6.5	1.0
FAR WAT ABS (%)	0.86	1.2	2.3	0.9
FAR STAB (sec)	0.90	52	104	1.0
Cookies width (cm)	0.86	0.23	0.39	1.1
Cookies height (cm)	0.91	0.03	0.06	1.0

The chemometric model based on PLS did not improve the results obtained for the technological traits.

Conclusions

Calibrations model performances were similar for einkorn whole meal and flour. The predictive ability of NIR models was good for moisture and protein content, satisfactory for SDS sedimentation volume and poor for rheological properties. The application of NIR analysis on whole meal samples is recommended in order to facilitate germplasm screening and early generation selection of outstanding lines.

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