Determination of fibres (arabinoxylans, β-glucans), sterols and alkylresorcinols in cereals and their fractions with NIR techniques

Short summary

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Introduction

In HEALTHGRAIN 150 wheat varieties and 50 varieties of rye, barley and oats, grown on one location and analysed for a range of dietary fibres and phytochemicals followed by growing and analysing 31 varieties at 4 locations. This included both wet chemical analysis and fast, non-destructive NIR analysis. The investigated big sample sets covered commodities (winter wheat, spring wheat, rye, oat, barley), crop year (three years), GxE (4 growing locations, 31 varieties) and instrument variations in order to maximise the robustness of calibration models.

Results

The statistical characteristics of optimised calibration models including all commodities are summarised in Table 1.

Table 1. Results of mPLS calibrations calculated with repeatability file.

Constituent	Number of samples	Range*	Mean*	Std. dev.*	RSQ	SEC*	SECV*	Terms
TOTAX in bran	353	3.83 – 22.60	16.259	3.280	0.849	1.276	1.325	10
WEAX in bran	353	0.15 – 1.53	0.489	0.244	0.833	0.099	0.108	13
TOTAX in flour	352	1.05 – 4.31	2.061	0.481	0.771	0.230	0.236	13
WEAX in flour	352	0.15 – 1.94	0.579	0.294	0.712	0.158	0.160	11
Total AR in whole meal	347	32.2 – 1444.0†	538.9†	214.8†	0.703	117.0†	123.0†	12
Total Sterols in whole meal	352	567 – 1276‡	780.5‡	117.4‡	0.803	52.1‡	53.8‡	12
Glucan in whole meal	352	0.24 – 6.54	0.966	0.964	0.917	0.278	0.317	13

* : % of dry weight, except † : µg/g of dry weight, ‡ : µg/g of fresh weight

The calibration models for total arabinoxylans (TOTAX), water extractable arabinoxylans (WEAX), alkylresorcinols and sterols provide fast and reliable routine screening methods, providing either quantitative or semi-quantitative results.

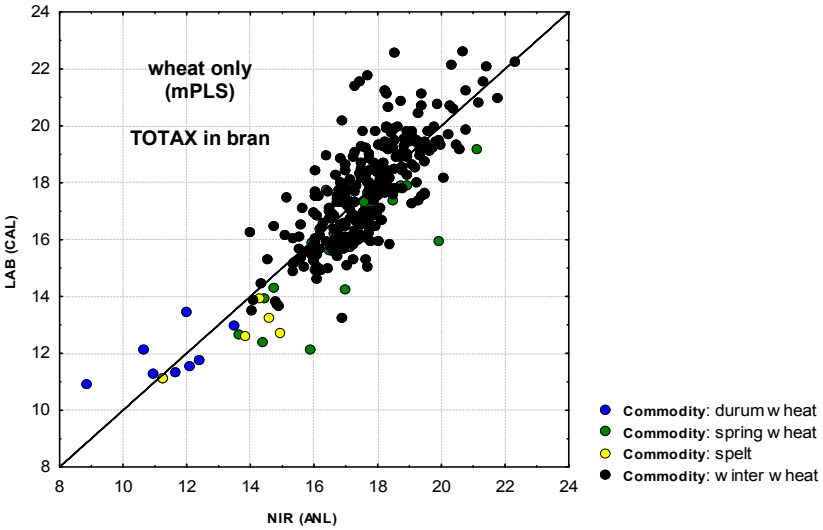
(Note: The apparently good calibration model of glucan in whole meal samples is reflecting a strong commodity effect; in spite of acceptable statistical results this model does not measure the concentration of glucan properly, so the model is ranking only the different commodities based on their glucan level).

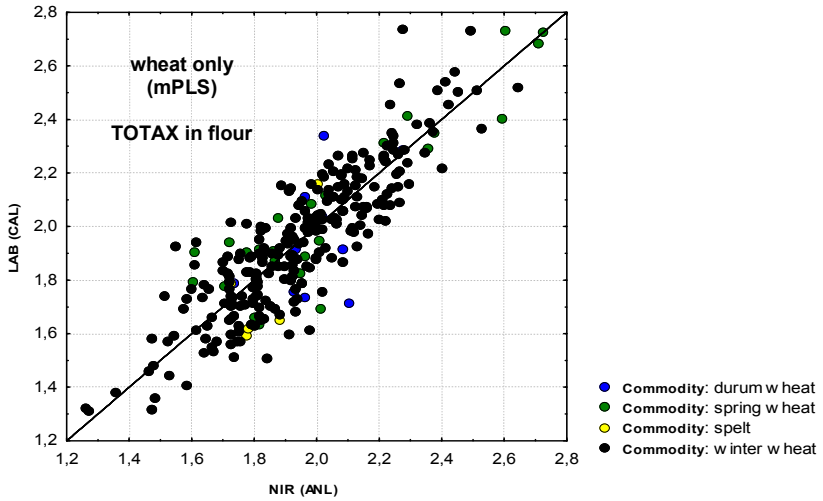
Statistical characteristics of separate calibration models developed for **wheat samples** only are summarized in Table 2 and visualized in the scatter plots below.

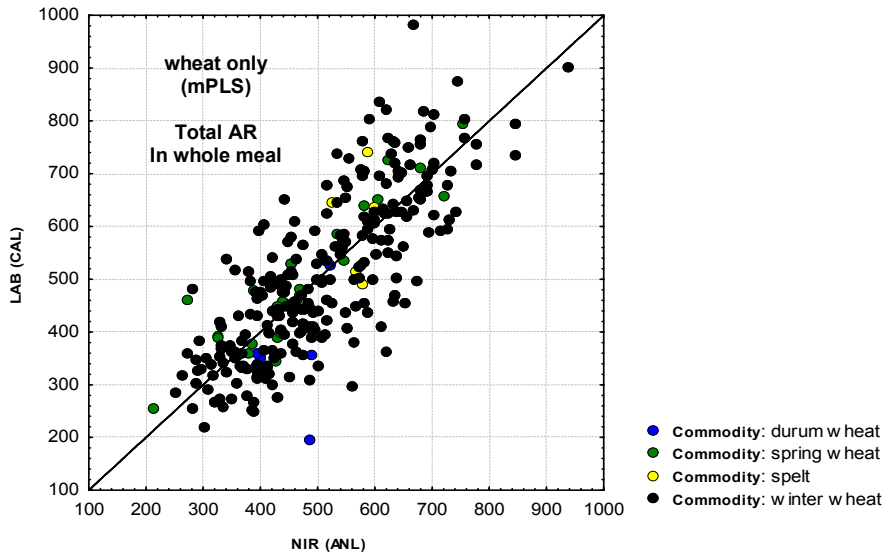
Table 2. Results of mPLS calibrations calculated using wheat samples.

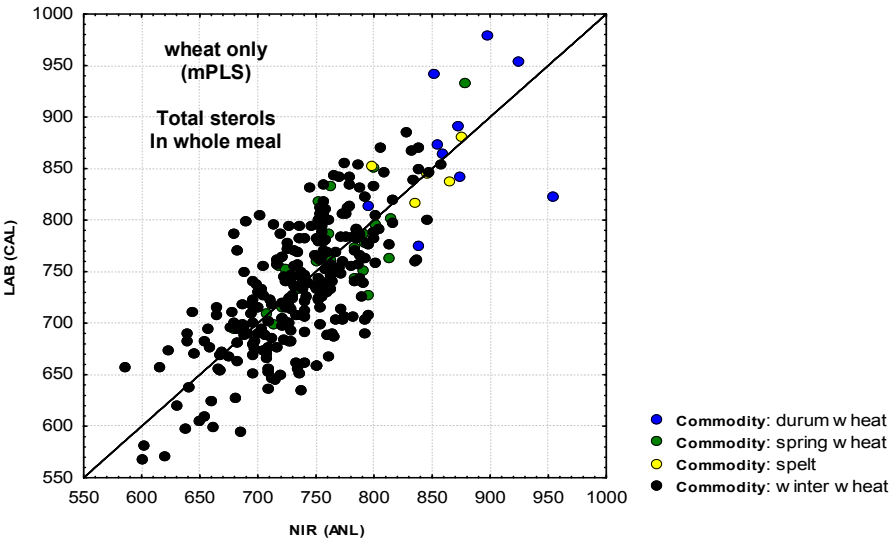
Constituent	Number of samples	Range*	Mean*	Std. dev.*	RSQ	SEC*	SECV*	Terms
TOTAX in bran	293	10.89 – 22.60	17.317	2.197	0.713	1.176	1.247	9
WEAX in bran	293	0.27 – 0.92	0.427	0.092	0.515	0.064	0.071	10
TOTAX in flour	293	1.31 – 2.74	1.952	0.270	0.822	0.114	0.132	13
WEAX in flour	293	0.24 – 1.07	0.514	0.141	0.452	0.104	0.115	8
Total AR in whole meal	292	194.3 – 981.0†	505.3†	151.5†	0.700	83.1†	91.6†	11
Total Sterols in whole meal	292	568 – 980‡	744.4‡	67.2‡	0.663	39.0‡	43.2‡	11
Glucan in whole meal	292	0.24 – 0.96	0.673	0.117	0.552	0.08	0.09	12

* : % of dry weight, except † : µg/g of dry weight, ‡ : µg/g of fresh weight









The dedicated models have poorer R-square values (compared to general models) due to reduced total variance of spectroscopic data file and narrower ranges of reference values. The standard error of cross-validation (SECV) values were smaller (the accuracy increased) compared to general models because the avoiding of commodity effects. The optimal number of latent variables was also slightly decreased.
The developed models can be used for screening or routine analysis of bioactives in whole meal and/or in different milling fractions of wheat.

Applications - examples
These calibration models may be used by

- breeders, for assessment of the arabinoxylan level and type in seeds
- millers to evaluate the efficiency of separation and mixing procedures
- Food technologists to select milling products or fractions for manufacturing products (with dedicated functional properties) with designed composition of bioactives.

.The models are transferable between different instruments. Validation process are needed following the calibration transfer.

Properties and performance of arabinoxylans, betaglucans, sterols and alkylresorcinols

The worldwide trend towards healthier eating and healthier products is leading in the cereal grain and bakery products area to a growing market share of whole grain products and products high in dietary fibre. Interest is growing in related areas, such as products high in arabinoxylans, the main fibre component in wheat and rye, and products with high levels of health promoting phytochemicals - the bioactive co-passengers of dietary fibre in whole grain- and related products.
In recent European and global regulations and recommendations on labelling products can only be labelled as 'source of fibre' or 'high in fibre' when the level of total fibre is at least 3% or 6%.
For **β-glucans** of oats and barley the health benefit - *contributing to maintaining normal blood cholesterol concentrations* - has been approved by EFSA (01-10-2009).
Arabinoxylans are the main fibre source of wheat and rye - wheat and rye fibres being unsurpassed in maintaining a regular intestinal function. The level and type of arabinoxylans (AX) has impact on technological performance as well - for instance soluble (water extractable) WEAX) is seen as more favourable than insoluble AX for bread baking purposes.
Sterols are well known for their cholesterol lowering effects.
Alkylresorcinols are markers of whole grain content of wheat and rye products.
The quantitative measurements of these bioactive compounds - total and soluble arabinoxylans, sterols and alkylresorcinols needs complicated wet chemical methods including laborious (extraction, saponification, purification, derivatisation separation, detection etc.) steps which are time consuming and expensive.

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