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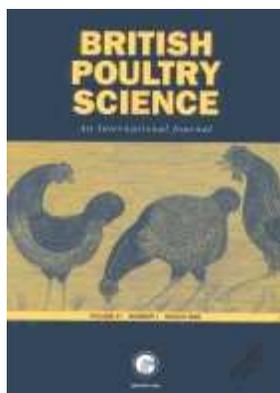
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Prediction of the chemical and physical characteristics and nutritive value of wheat by near infrared reflectance spectroscopy

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10 **Prediction of wheat chemical and physical characteristics and nutritive value by near-**
11 **infrared reflectance spectroscopy**
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36 **RUNNING TITLE: PREDICTING WHEAT CHARACTERISTICS WITH NIRS**
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56 **Accepted for publication 18th August 2008**
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2
3 **Abstract** 1. The aims of this study were to investigate the potential of near infrared reflectance
4 spectroscopy (NIRS) to predict the chemical and physical characteristics of wheat and also to
5 predict the nutritive value of wheat for broiler chickens.
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10 2. A total of 164 wheat samples, collected from a wide range of different sources (England,
11 Northern Ireland and Canada), varieties and years, were used in this study.
12

13 3. Chemical and physical parameters measured included specific weight, thousand grain weight,
14 *in vitro* viscosity, gross energy, nitrogen, neutral detergent fibre (NDF), starch, total and soluble
15 non-starch polysaccharides (NSP), lysine, threonine, amylose, hardness, rate of starch digestion
16 and protein profiles.
17
18

19 4. A total of 94 wheat samples were selected for inclusion in three bird trials and included at
20 650g/kg in a typical UK starter/grower diet. Birds were housed in individual wire metabolism
21 cages from 7-28 d and offered water and food *ad libitum*. Dry matter intake (DMI), live weight
22 gain (LWG) and gain:feed ratio were measured weekly. A balance collection was carried out
23 from d 14 - d 21 for determination of apparent metabolisable energy (AME), ME:gain and dry
24 matter retention. At 28 d the birds were humanely killed, the contents of the jejunum removed
25 for determination of *in vivo* viscosity and the contents of the ileum removed for determination of
26 ileal dry matter, starch and protein digestibility.
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30 5. The wheat samples were scanned as whole and milled wheat, both dried and undried and NIRS
31 calibrations, first excluding and then including the Canadian wheat samples, were developed.
32
33

34 6. NIRS calibrations for milled wheat samples may be useful for determining specific weight
35 ($R^2_{cv} = 0.75$, for milled wheat dried), nitrogen ($R^2_{cv} = 0.983$ for milled and dried) and rate of
36 starch digestion ($R^2_{cv} = 0.791$ for milled, dried and undried).
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3 7. NIRS calibrations for whole wheat samples (undried) may be useful for determining wheat
4 nutritive value, with good predictions for live weight gain ($R^2_{cv} = 0.817$) and feed conversion
5 efficiency ($R^2_{cv} = 0.825$).
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10 8. Inclusion of the Canadian wheat samples in the NIRS analysis provided additional robust
11 calibrations for gross energy ($R^2_{cv} = 0.86$, dried and milled) and starch content ($R^2_{cv} = 0.79$,
12 undried and milled).
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17 8. This study shows that NIR is a useful tool in the accurate and rapid determination of wheat
18 chemical parameters and nutritive value and could be extremely beneficial to both the poultry and
19 wheat industry.
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24 9. Further extension of the dataset would be recommended to further validate these findings.
25
26

27 INTRODUCTION

28
29 Wheat is an important component of poultry diets. The chemical and structural properties of
30 wheat are not constant, and there can ultimately be significant variation in feed intake and
31 performance by animals and birds offered wheat-based diets. Rose *et al.* (1993), Scott *et al.*
32 (1998) and McCracken and Quintin (2000) all reported a range of over 10% in the growth rates of
33 chickens fed on different wheat samples. Internationally, specific weight continues to be used as
34 a measure of feed wheat quality, despite reports showing a lack of a relationship between specific
35 weight and nutritive value for poultry (Wiseman, 2000; Miller *et al.*, 2001; McCracken *et al.*,
36 2002). There is therefore a clear need for an alternative, accurate and rapid method of assessing
37 wheat quality.
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50 The chemical analysis of wheat is time consuming and costly and the assessment of
51 nutritive value *in vivo* is considerably more time consuming, expensive and also requires
52 specialised resources (Garnsworthy *et al.*, 2000). A more beneficial method would be near-
53 infrared spectroscopy (NIRS), which is routinely used in the flour milling industry for the rapid
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3 determination of moisture and protein in wheat and is now used to predict the nutritive value of
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5 forage for ruminants (Park *et al.*, 1998).
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8 Garnsworthy *et al.* (2000) found that NIRS could accurately estimate the chemical
9
10 composition and agronomic characteristics of wheat, but accurate prediction of nutritive value
11
12 from chemical or agronomic characteristics were very inaccurate (coefficients of determination
13
14 varied from zero to 0.25). Rose *et al.* (2001) found NIRS useful for determining endosperm
15
16 hardness and suggested it has the potential as a rapid test of nutritional value for wheat samples
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18 arriving at poultry feed mills.
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22 The main objectives of this study were to investigate the potential of NIRS to predict the
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24 chemical and physical characteristics of wheat and also to predict the nutritive value of wheat for
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26 broiler chickens.
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29 MATERIALS AND METHODS

30 **Animal ethics**

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32 This study was conducted according to the Animals (Scientific Procedures) Act 1986 and was
33
34 approved by the Newforge Ethical Committee.
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38 **Sample collection**

39
40 The 164 wheat samples used in this study were gathered over a wide range of different locations,
41
42 varieties and years. A total of 62 of the wheat samples were taken from Miller *et al.* (2001). By
43
44 analysing these older samples for total starch, crude protein and dry matter content we ensured
45
46 the samples had not deteriorated over time. Of these, 30 were from the 1998 harvest from
47
48 Northern Irish plant testing sites at Crossnacreevy, Downpatrick and Limavady (10 varieties:
49
50 Cantata, Ritmo, Riband, Chaucer, Reaper, Brigadier, Madrigal, Hussar, Harrier and Equinox
51
52 from each site). The other 32, from this study reported by Miller *et al.* (2001), consisted of eight
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54 1999 Northern Ireland varieties (Aardvark, Charger, Hereward, Reaper, Equinox, Napier, Rialto,
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3 Savannah and Consort) from two plant testing sites (Downpatrick and Limavady) and 16 wheats
4 from Great Britain (GB), of 4 different varieties (Buster, Consort, Riband and Haven) at 4 levels
5 of specific weight. In addition, 10 samples: Claire, Consort, Malacca, Tanker, Napier, Savannah,
6 Aarvark, Rialto, Riband and Soissons; were collected from each of the 2003 and 2004 harvests at
7 Crossnacreevy, Northern Ireland. Another 20 samples: Claire, Consort, Malacca, Tanker,
8 Soissons, Riband, Napier, Goodwood, Savannah and Vector, at high and low nitrogen levels (180
9 kg N/ha and 260 kg N/ha), were collected from the 2005 harvest at Crossnacreevy. Another 30
10 samples were taken from HGCA Project 2979 entitled "GREEN Grain" currently being
11 undertaken by ADAS. Ten samples were obtained from shipments from GB containing
12 commercial wheat samples for Moy Park Limited (Dungannon, Northern Ireland) and the
13 remaining 22 samples were sourced from Canada (Pacific Agri-Food Research Centre, Agassiz,
14 B.C.).

31 Diets

32
33 Of the above wheat samples, 94 were selected for inclusion in three animal trials. By exactly
34 replicating the design from Miller *et al.* (2001), results for 32 wheat samples from this previous
35 animal trial were combined with results from three animal trials (62 wheat samples) in the present
36 study. Wheats were selected to give as wide a range of bird performance results as possible.
37 Insufficient Canadian wheat sample was available for inclusion in the experimental diets. Wheat
38 was ground in a hammer-mill using a 5 mm screen. The diet formulation (Table 1) was a typical
39 UK starter/grower with a small inclusion of lysine, threonine and methionine to equalise these
40 across all diets based on amino acid analysis of the wheat samples. Titanium dioxide was added
41 as an indigestible marker. The diets were mixed, heat treated (80°C, 90 s) and pelleted (3 mm
42 die) at the Agri-Food and Biosciences Institute, Belfast.

Table 1 near here

57 *Experimental design*

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2
3 The first broiler trial investigated 20 wheat samples, 10 from each of the 2003 and 2004
4 Crossnacreevy harvest. A total of 60 birds were used in each of three replicates (9
5 birds/treatment), with three weight blocks of 20 in each replicate. All 20 treatments were
6 randomly allocated within a weight block of 20 birds. The second broiler trial investigated 32
7 wheat samples selected from the 2005 Crossnacreevy harvest, HGCA Project 2979 and GB
8 commercial samples. A total of 64 birds were used in each of 5 replicates (10 birds/treatment),
9 with two weight blocks of 32 in each replicate. All 32 treatments were randomly allocated within
10 a weight block of 32 birds. The third trial investigated 10 wheat samples selected from the 2005
11 Crossnacreevy harvest and HGCA Project No. 2979. A total of 60 birds were used in each of two
12 replicates (12 birds/treatment), with 6 weight blocks of 10 in each replicate. All 10 treatments
13 were randomly allocated within a weight block of 10 birds.
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29 **Birds and management**

30 For each experimental replicate, 100 male Ross broiler chicks from 30-40 week old breeders and
31 one breeder farm were obtained at hatching from Moy Park Ltd. (Dungannon, Northern Ireland).
32 They were placed in a commercial brooder for 7 d with *ad libitum* access to water and a crumbled
33 starter diet (Hi-Grain Chick Crumbs, John Thompson and Sons, Belfast). At 7 d, all birds were
34 weighed and the heaviest and lightest discarded, leaving a sufficient number so that the birds
35 could be allocated to experiment according to the randomisation. Birds were placed in individual
36 wire metabolism cages at an initial room temperature of 33°C, reduced by 1°C every 2 d down to
37 24°C. The light:dark cycle was 18:6 and relative humidity was set at 50%. Birds were offered
38 water and food *ad libitum* from d 7 – d 28, with dry matter intake, live weight gain and gain:feed
39 being recorded on a weekly basis.
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55 The balance procedure for determination of apparent metabolisable energy was carried
56 out from d 14 – d 21. The individual bird excreta were collected daily and stored at 4°C. At the
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3 end of the balance week the excreta were weighed and then oven-dried at 80°C. The sample
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5 weights were allowed to equilibrate and the sample was then milled through a hammer mill fitted
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7 with a 0.75 mm screen and stored for subsequent analysis. At 28 d, the birds were humanely
8
9 killed by dislocation of the spinal cord and the contents of the proximal jejunal removed for
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11 determination of *in vivo* viscosity and the contents of the ileum collected to determine ileal
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13 digestibility.
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16 17 **Analysis of wheat samples, diets, excreta and ileal digesta**

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19 The wheat samples were analysed for dry matter, specific weight, thousand grain weight, *in vitro*
20
21 viscosity, gross energy, nitrogen (N), neutral detergent fibre (NDF), starch, total and soluble non-
22
23 starch polysaccharides (NSP), lysine, threonine, amylose, hardness, rate of starch digestion and
24
25 protein profiles. The diets were analysed for titanium dioxide, dry matter, crude protein (N ×
26
27 6.25), crude fat, NDF, ash, starch and gross energy. The excreta samples were analysed for dry
28
29 matter and gross energy. The ileal digesta were analysed for dry matter, titanium dioxide, crude
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31 protein (N × 6.25) and starch. All analyses were carried out in duplicate and results reported on a
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33 dry matter (DM) basis.
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39 Dry matter was determined by oven drying at 100°C for 24h and ash content was
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41 determined by ashing samples in a muffle furnace at 450°C for 16 h (AOAC, 1990). Specific
42
43 weight was measured using a Digi-sampler hectolitre test weight machine (ELE International
44
45 Limited), and thousand grain weight by using a Numigral seed counter (Tecator Ltd, Sweden)
46
47 and measuring the weight of 1000 grains in duplicate. *In vitro* viscosity was determined using a
48
49 modification of the method described by Bedford and Classen (1993). The digesta were
50
51 centrifuged (13400 g for 8 min) and viscosity measured using a Brookfield LVDV II cone and
52
53 plate viscometer at 20°C. Nitrogen was determined using the LECO FP-2000 dry combustion
54
55 analyser (Leco Corporation, Michigan, USA) and oil B by acid hydrolysis (3M HCl), followed
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3 by solvent extraction with petroleum ether (40-60°C) in a Soxtec system (Stoldt, 1952). NDF
4
5 was determined using the Fibertec system (Tecator Ltd, UK) according to the method of Van
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7 Soest (1963). Cold NDF reagent (sodium dodecyl sulphate, EDTA disodium salt,
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9 $\text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$, Na_2HPO_4 and 2-ethoxyethanol and water) and enzyme solution (amylase, BDH,
10
11 cat. no. 39004) were added to the sample, then boiled and dried. Total starch was determined
12
13 using a commercial enzyme assay kit (Megazyme International Ireland Ltd) as described by
14
15 McCleary *et al.* (1997). Total and soluble NSP content were determined using a commercial
16
17 enzyme assay kit as described by Englyst *et al.* (1994). Amino acid content was determined,
18
19 following acid hydrolysis (6M HCl), on a Biochrom 20 amino acid analyser, using norleucine as
20
21 internal standard. Gross energy was determined using an isothermal automated bomb calorimeter
22
23 (PARR, Model 1271). Amylose content was determined using a commercial assay kit
24
25 (Megazyme International Ireland Limited), which is a modification of the procedure described by
26
27 Yun and Matheson (1990). The hardness of the wheat samples was firstly measured using a
28
29 single kernel characterisation system (SKCS) (Harper Adams University) and then repeated at
30
31 AFBI, Hillsborough, using a more recent version of the equation obtained from Campden
32
33 Chorleywood Food Research Association (CCFRA), Gloucestershire. Rate of starch digestion
34
35 was determined by the Englyst method (Englyst *et al.*, 1996). *In vitro* starch digestion follows
36
37 first-order kinetics, and *in vitro* starch digestion rate was estimated using the following equation:
38
39 $\text{DC}_t = D \cdot (1 - e^{-k(d) \cdot t})$, where DC_t is the starch fraction at time t and fraction D is the potentially
40
41 digestible starch fraction that will digest at a fractional rate of k_d (h^{-1}). This terminology was the
42
43 same as used by Weurding *et al.* (2001). The % starch at each time period was expressed as a
44
45 fraction of the maximum starch obtained from the above equation. Profiling of the protein
46
47 fractions was measured by electrophoretic and densitometric analysis and this was carried out by
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49 CCFRA. The detected bands were grouped into 5 major bands. These were, band 1: HMW-
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3 glutenin subunits, band 2: larger LMW-glutenin and ω -gliadin subunits, band 3: smaller LMW-
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5 glutenin and ω -gliadin subunits, band 4: α -, β -, γ -gliadin subunits and band 5: albumins and
6
7 globulins. Titanium dioxide content was determined by ashing the sample and then digesting
8
9 with concentrated sulphuric acid. Colour development was obtained with hydrogen peroxide and
10
11 absorbance measured by spectrophotometry (U-2010 spectrophotometer, Davidson and Hardy
12
13 Ltd) at wavelength 408nm.
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16 17 **Statistical analysis**

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19 The results of the animal trials were subjected to analysis of variance using Genstat Release 9.2,
20
21 with initial weight as a co-variate for growth parameters.
22

23 **Near Infrared Reflectance Spectroscopy (NIRS)**

24 *Preparation of wheat samples*

25
26 The milled wheat samples were milled through a hammer-mill (Cross Beater MK II, Glen
27
28 Creston Ltd, Middlesex, England) fitted with a 0.75 mm screen and stored in polyethylene jars
29
30 with metal screw caps and kept in the laboratory at room temperature. The dried wheat samples
31
32 were dried for 24 h in an oven at 100°C.
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34

35 *NIRS scanning*

36
37 The wheat samples were scanned on a Foss NIRSystems 6500 spectrophotometer (FOSS UK Ltd,
38
39 Warrington, UK). Samples were presented in a transport quarter cell for (a) undried and (b) dried
40
41 whole wheat samples and in a static ring cell for (c) undried and (d) dried milled wheat samples.
42
43 Two separate packings per sample were scanned at 2 nm intervals over the visible and near
44
45 infrared wavelength range, (*i.e.* 400 to 2500 nm) and the optical data recorded as log
46
47 1/Reflectance (log 1/R) values using the ISI-NIRS3 Version 4.00 (Infrasoft International, Port
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49 Matilda, PA, USA) software. The NIR spectra were subsequently trimmed to 1100-2498 nm
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51 before mathematical treatment of the data. Sub-sampling error was reduced by setting the root
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3 mean square (RMS) difference from the mean of each sub-sample at each wavelength to 700 and
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5 2000 μlog optical density (OD) for milled and whole kernel samples respectively.
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10 *Development of NIRS calibrations*

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13 The spectrum contains information about the chemical nature of the sample plus extraneous
14
15 noise. Mathematical first order derivation and Standard Normal Variate and Detrend (SNV-D)
16
17 (Barnes *et al.*, 1989) scatter correction procedure were applied as there is evidence that these
18
19 techniques can reduce spectral interference from particle size and other extraneous effects (Baker
20
21 and Barnes, 1990). Modified partial least squares (MPLS) regression technique (Martens and
22
23 Naes, 1989) was used to develop the NIRS calibrations. In the MPLS regressions, the spectral
24
25 data are reduced to a few independent factors, thus retaining most of the spectral information.
26
27 These independent factors were regressed against the reference laboratory data (*i.e.* SW, TG, *in*
28
29 *vitro* viscosity, N, NDF, starch, NSP, lysine, threonine, gross energy, amylose, rate of starch
30
31 digestion, hardness and protein profiles) and animal performance data (*i.e.* DMI, LWG, G:F, *in*
32
33 *vivo* viscosity, ME:GE, AME content, ME:Gain, DM retention and ileal DM, starch and protein
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35 digestibility).
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42 When developing MPLS equations, cross-validation was used to select the optimum
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44 number of factors and so avoid over-fitting which occurs where the R^2 continues to increase but
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46 the error for the calibration, after reaching a minimum value, also starts to increase as more
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48 factors are added. The number of factors was set at an upper limit of 11. Cross-validation
49
50 occurred by first splitting the populations into 6 groups, with one group removed in turn from the
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52 database until all 6 groups had been removed. Calibrations were formed using the remaining five
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54 groups, and the excluded group was then predicted. Validation errors were combined into a
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3 standard error of cross-validation (SECV) and the optimum number of factors was taken as the
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5 number resulting in the lowest prediction error. The datasets for each wheat type (milled –
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7 undried and dried; kernels – undried and dried) were then split randomly taking every 5th sample
8
9 to form a true validation set and the remaining 4/5 were used to develop a calibration for each
10
11 parameter (we shall call these sub-calibrations). The validation sets were then predicted using the
12
13 respective sub-calibration set and the results compared to the actual laboratory and animal data.
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17 The Standard Error of Prediction (SEP) was calculated as: $SEP = \sqrt{[\sum (D)^2] / n}$
18

19
20 Where D = the difference between the reference value and the predicted
21
22 value.
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25 The NIR equation statistics were performed with and without the Canadian wheats (on
26
27 milled samples only).
28

29 RESULTS

30 *Chemical and physical analysis of wheat samples*

31
32 The minimum, maximum and mean values from the chemical and physical analysis of the wheat
33
34 samples are shown in Table 2. Unfortunately, problems occurred with both the hardness
35
36 methods. The first method could not incorporate all the wheat samples as they were not available
37
38 and also more recent and accurate methods are available. For the second method, the SKCS
39
40 NIRS equation, which was developed at CCFRA, was skewed and biased in order to predict
41
42 samples scanned on the NIRSystems 6500 instrument at AFBI, Hillsborough. However, we
43
44 cannot be certain that the results obtained from the adjusted SKCS equation are correct as the H
45
46 value (Mahalanobis distance) is not affected by skewing and biasing, only the predicted results.
47
48 Therefore the H value was large (average H value of 35.04). Normally the H value should be less
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50 than 3, indicating that the samples are similar to those in the sample database.
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Table 2 near here

Animal trials

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3 Unfortunately, one of the diets had to be eliminated from the third animal trial due to water
4 damage during storage (Spark, -N, High Mowthorpe). Therefore, results are only reported for the
5 remaining 93 wheat samples used in the animal trials (Table 3).
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Table 3 near here

10
11 When the three animal trials from this study were combined with the results of Miller *et*
12 *al.* (2001), it was found that there were very highly significant ($P<0.001$) differences between
13 diet treatments for all the measured parameters (total DMI, LWG and gain:feed, *in vivo* viscosity,
14 ME:GE, AME content, ME:Gain, dry matter retention, ileal dry matter, starch and protein
15 digestibility). Total DMI ranged from 61.6 (Ambrosia, -F, HM) to 85.7 g/d (Buster 71, 1998/99,
16 total LWG ranged from 41.9 (Ambrosia, -F, HM) to 64.2 g/d (Buster 71, 1998/99) and total
17 gain:feed ranged from 0.67 (Predator, -N, Terr) to 0.82 (Riband, 2004). *In vivo* viscosity ranged
18 from 3.3 (Riband, 2003) to 13.0 cps (Malacca, high N, 2005), ME:GE ranged from 0.67 (Buster
19 67, 1998/99) to 0.78 (Predator, -N, HM) and AME content ranged from 12.67 (Buster 67,
20 1998/9) to 14.79 MJ/kg (Malacca, high N, 2005). ME:Gain ranged from 16.72 (Soissons, high N,
21 2005) to 20.86 MJ/kg (Zebedee -N, Terr), dry matter retention ranged from 0.70 (Napier, S/R
22 640, Rose) to 0.75 (Napier, high N, 2005) and ileal dry matter ranged from 0.63 (Claire, high N,
23 2005) to 0.76 (Consort, 2003)). Starch digestibility ranged from 0.83 (Aardvark, 2004) to 0.97
24 (Goodwood, low N, 2005)) and ileal protein digestibility ranged from 0.70 (Consort, high N,
25 2005) to 0.83 (Savannah, 2004).
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45 NIRS

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47 *Full calibrations based on all wheats but excluding Canadian wheats*

48 Table 3 presents the range, standard deviation and number of samples analysed for each
49 parameter using all the wheat samples but excluding the Canadian wheat. Tables 4(a), 5(a), 6(a)
50 and 7(a) present the statistics for the calibrations developed for each parameter using the full
51 database, excluding the Canadian wheat. Overall good NIRS calibrations with high R^2 and low
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errors (SEC) were produced for the majority of parameters across all sample types. Milled wheat samples typically produced better correlation statistics as the sample is more homogeneous than the whole kernel wheat samples. Standard error of cross validation (SECV) and the corresponding coefficient of determination of cross validation (R^2_{cv}) are the statistics which better reflect how the calibration will perform when predicting unknown wheat samples. SECV expressed as a percentage of the mean reference value is presented to give a clearer indication of the error associated with the prediction equations. Ideally percentage error would be $\leq 2\%$ for laboratory analyses. Biological parameters are much more difficult to estimate and therefore larger errors are acceptable. NIRS errors are typically greater than the errors associated with the reference method. Dried milled wheat samples, yielded some strong calibrations, with high R^2 for SW (0.82), TG (0.75), *in vitro* viscosity (0.79), N (0.99), starch (0.78), total NSP (0.77), threonine (0.77), GE (0.82), RSD (0.125h) (0.84), RSD (0.250h) (0.87), RSD (0.375h) (0.87), RSD (0.5h) (0.83), RSD (0.75h) (0.83), RSD (1h) (0.83), RSD rate constant (0.83), hardness (0.87), protein profile bands 1 (0.83), 2 (0.87), 3 (0.76) and 4 (0.88), ME:GE (0.79), AME content (0.72) and ME:Gain (0.88). Good cross validation statistics, $R^2_{cv} \geq 0.75$ were achieved for SW (0.75), N (0.98), GE (0.76), RSD (0.125h) (0.81), RSD (0.250h) (0.80), RSD (0.375h) (0.80), RSD (0.5h) (0.77), RSD (0.75h) (0.78), RSD rate constant (0.78), hardness (0.79) and protein profile bands 1 (0.75), 2 (0.78), 4 (0.77) and ME:gain (0.78) (Table 4(a)).

Tables 4,5,6,7 near here

The NIR equation statistics for the undried milled wheats (Table 5(a)) also achieved good correlations similar to the dried wheats with R^2 values for SW (0.80), TG (0.77), N (0.99), starch (0.77), threonine (0.80), GE (0.86), RSD (0.125h) (0.87), RSD (0.250h) (0.86), RSD (0.375h) (0.79), RSD (0.5h) (0.84), RSD (0.75h) (0.80), RSD (1h) (0.78), RSD rate constant (0.81) and protein profile bands 1 (0.84), 2 (0.78), 4 (0.92) and 5 (0.85), 7-14d DMI (0.82), 7-14d LWG (0.86), 14-21d LWG (0.83), 21-28d LWG (0.82), total LWG (0.84), 14-21d gain:feed (0.81),

total gain:feed (0.84) and ME:Gain (0.82). High R^2_{cv} results were still achieved for N (0.98), RSD (0.125h) (0.83), RSD (0.250h) (0.83), RSD (0.375h) (0.77), RSD (0.5h) (0.79), RSD (0.75h) (0.76), RSD rate constant (0.80), protein profile band 4 (0.86) and 7-14d LWG (0.75).

Tables 6(a) and 7(a), presenting the calibration statistics for the dried and undried whole wheat, show that fewer calibrations produced $R^2_{cv} \geq 0.75$ when their spectra were regressed against the reference data for the chemical and physical parameters. Of particular interest are the biological parameters, DMI, LWG and gain:feed, which produced robust calibrations (R^2_{cv} ranging from 0.76 - 0.83 and corresponding SECV as percentage of the mean from 2.35 - 6.50%) for the undried whole kernel wheats, which is the natural state that we would wish to use routinely to predict chemical composition and feed value.

Independent validation using a NIRS sub-calibration (excluding Canadian wheats)

In order to assess fully the NIRS calibrations, sub-calibrations were developed for each sample type, based on randomly selecting 4/5 of the database and these sub-calibrations were then used to predict the remaining 1/5 of samples. The reference values for the independent samples and the NIRS predicted values were compared and the standard error of prediction (SEP) calculated. Tables 4b, 5b, 6b and 7b show the sub-calibration and the true validation statistics for each parameter. Nitrogen prediction equations performed strongly for all wheat types with R^2 values ranging from 0.82 for undried whole wheat to 0.91 for dried milled wheat and SEP values of 1.03 - 0.65 respectively. Figure 1 shows a regression plot of the dried and undried milled wheat nitrogen predictions versus the reference values. The validation results for dried milled wheats show that the NIRS sub-calibrations performed well for nitrogen, total NSP, threonine, GE, RSD (0.125, 0.25, and 0.375h), RSD rate constant and protein band 1 and 4, with R^2 of 0.91, 0.71, 0.70, 0.82, 0.75, 0.70, 0.70, 0.74, 0.75, and 0.77 respectively. The SEP expressed as a percentage

Figure 1 near here

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3 of the mean ranged from 0.22% for GE to 12.9% for the RSD rate constant which would be a
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5 difficult measurement.
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8 SW, TG, starch, amylose, RSD (0.5, 0.75 and 1h), ME:GE and ileal starch digestibility all
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10 produced correlations $R^2 > 0.60$ and SEP as % of mean of 3.67, 10.85, 3.60, 4.82, 6.78, 5.25, 3.61,
11
12 2.31 and 4.79 respectively. These results are very encouraging and additional wheat samples
13
14 may improve the calibrations. Similar results were observed for the undried milled wheats.
15
16 Regression plots of actual and predicted RSD rate constant for dried and undried milled wheat are
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18 presented in Figure 2.
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Figure 2 near here

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23 Whole dried wheat validations only produced good correlations ($R^2 > 0.60$) for SW,
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25 nitrogen, total LWG and ileal DM digestibility although low SEP % errors of 3.16, 0.43, 4.66,
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27 2.64, 5.47, 7.20, 4.60, 1.93, 3.74, 2.90, 3.58, 2.78 for starch, GE, RSD (1h), RSD(2h), total DMI,
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29 total LWG, total gain:feed, ME:GE. ME:gain, ileal DM digestibility, ileal starch digestibility and
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31 ileal CP digestibility would indicate the potential to improve these equations. In most cases
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33 similar or poorer relationships were found with undried whole wheat comparisons. However, for
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35 total gain:feed very good calibrations ($R^2 = 0.75$) were observed for undried whole wheat with
36
37 low SEP percentage errors of 3.19%. Figures 3 and 4 show the validation statistics when LWG
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39 and total gain:feed reference and predicted values were compared for dried and undried whole
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44 wheat.

Figures 3 and 4 near here

45 46 *Full calibrations based on all wheats including Canadian wheats*

47
48 Canadian wheats had been analysed for TG, *in vitro* viscosity, nitrogen, NDF, starch, GE, RSD
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50 (0.125, 0.250, 0.375, 0.50, 0.75, 1 and 2h, and RSD rate constant. The spectral data for dried and
51
52 undried milled wheats plus the reference data for the Canadian wheats were added to the original
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54 dried and undried databases and full calibrations produced. Table 8 shows the total number of
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56 samples, the range and standard deviation of the parameters used to develop the new NIRS
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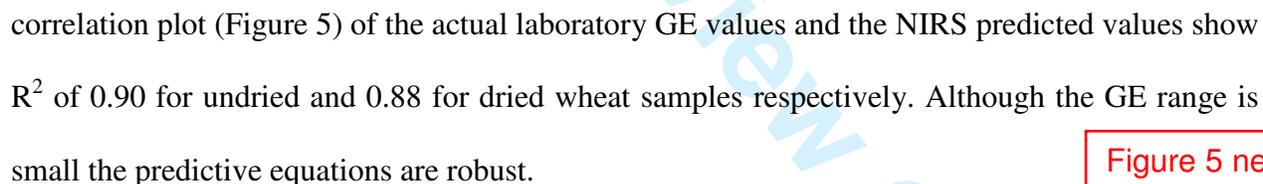
Tables 8,9,10 near here

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3 calibrations. The calibration statistics for the dried and undried milled wheats are presented in
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6 Tables 9(a) and 10(a) respectively.

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8 Including the Canadian wheat samples produced good predictive equations with high R^2
9
10 and very good R^2_{CV} values for almost all parameters for both dried and undried milled wheats.
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12 However, *in vitro* viscosity appears to be a poor equation with SECV as % of the mean of 26.28
13
14 and 25.09% for dried and undried samples respectively.

15 16 17 *Independent validation using a NIRS sub-calibration including the Canadian wheats*

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19 Again sub-calibration databases including the Canadian wheats were randomly selected and the
20
21 equations produced predicted the remaining 1/5 of samples excluded from the calibration. The
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23 calibration statistics for the sub-calibration and true validation statistics are presented in Tables
24
25 9(b) and 10(b). Both the dried and undried validations produced fairly good correlations $R^2 > 0.60$
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27 for nitrogen, GE, RSD digestibility parameters and the RSD rate constant. SEP % errors are
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29 particularly low for nitrogen, starch, GE, RSD (0.75, 1 and 2h) ranging from 0.28 – 5.32. A
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31 correlation plot (Figure 5) of the actual laboratory GE values and the NIRS predicted values show
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33 R^2 of 0.90 for undried and 0.88 for dried wheat samples respectively. Although the GE range is
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35 small the predictive equations are robust.

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41 In summary, the milled samples, dried and undried, produced good calibrations for SW,
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43 N, RSD, hardness, and some of the protein bands. The whole wheat samples, dried and undried,
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45 produced good calibrations for N, LWG and gain:feed. By including the Canadian wheat,
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47 additional strong calibrations were obtained for GE and starch content.

50 DISCUSSION

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52 Many papers discussing NIRS do not go beyond the internal calibrations carried out initially in
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54 this study. Therefore any calibrations considered strong after an independent validation with a
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56 separate set of samples in this study can be considered more robust than those reported by others.
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3 A coefficient of cross validation (R^2_{cv}) greater than 0.75 is accepted by industry, as an indicator
4 that a strong calibration has been achieved for predictive purposes. The errors (SECV and SEP)
5 associated with the predictions have to be taken into consideration as high correlations alone may
6 sometimes be misleading. Only by taking into account both correlation and error statistics can
7 one decide if the equation is acceptable for the parameter of interest. Laboratories usually accept
8 2-3% error for repeatability while errors associated with biological parameters will be higher.
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17 In general, NIRS calibrations for the chemical parameters of wheat were best predicted by
18 the milled wheat samples, while calibrations for the nutritive value of wheat were best predicted
19 by the whole wheat samples. The calibrations for specific weight were good for the dried wheat
20 samples, with the calibration for milled dried wheat being stronger, producing a coefficient of
21 cross validation of 0.747 and a 2.72 % error of cross validation. The determination of protein
22 content in wheat is historically the most important application of NIR analysis and NIR is now
23 widely used for this purpose in the flour milling industry (Osbourne *et al.*, 1993). In the current
24 study, the nitrogen content of the wheat samples was well predicted by all forms of wheat.
25 Unsurprisingly, the milled and dried wheat had the highest coefficient of cross validation (0.983),
26 with only a 1.63% error of cross validation. This compares favourably with Garnsworthy *et al.*
27 (2000), who reported a standard error of cross validation of 0.89. The rate of starch digestion is
28 well predicted using NIRS, but only on the wheat that was milled. Coefficients of cross
29 validation from 0.699 - 0.829 were achieved when predicting the amount of starch digested at
30 7.5, 15, 22.5, 30, 45 and 60 minutes and 0.791 when predicting the rate of starch digestion. This
31 result is particularly exciting as the determination of the rate of starch digestion is a costly and
32 time consuming analysis and therefore a quick and reliable method would be well received. A
33 possible explanation for the calibrations being strong in the milled wheat samples, but not in the
34 whole kernel, is that the particle size of ground wheat has a significant effect on starch
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3 digestibility. It is generally thought that smaller particles with an increased surface area will
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5 allow increased access to digestive enzymes and enhance digestion of nutrients (Waldroup,
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7 1997). Péron *et al.* (2005) reported positive effects of fine grinding of wheat on starch
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9 digestibility. Calibrations for NDF, total NSP and soluble NSP were weak, the highest
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11 coefficients of cross validation being 0.54, 0.69 and 0.48 respectively. The calibrations for starch
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13 and amylose were not as good as would be expected for chemical parameters with R^2_{cv} of 0.711
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15 and 0.632 respectively for milled and dried wheat. Garnsworthy *et al.* (2000) also produced
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17 similar calibrations for starch (0.74) and speculated that because starch is not a single entity,
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19 differences occur in the size of starch granules and their interaction with the protein matrix of the
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21 endosperm may cause interference with the spectral patterns.
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27 Gross energy also produced a good calibration in the current study, the highest R^2_{cv} being
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29 0.760 for milled wheat undried. This may have been improved if the variation in the reference
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31 values (18.09-18.84 MJ/kg DM, without Canadian wheat) had been greater. As expected, the
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33 coefficients of cross validation of ME:GE and AME content were poorer (0.683 and 0.608
34
35 respectively) than for gross energy, as they were also subject to animal variation. Prediction of
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37 the different bands of proteins seems possible when observing the R^2_{cv} values ranging up to 0.86.
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39 However, the corresponding errors of cross validation as a percentage of the mean, reached as
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41 high as 13.15%. This is a relatively large error and therefore may render the use of the
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43 calibration for the prediction of protein bands as impractical.
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48 For the first time, good predictions for live weight gain and feed conversion efficiency
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50 were achieved using the undried whole wheat samples ($R^2_{cv} = 0.817$ and 0.825 respectively).
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52 This could have major benefits to the feed wheat industry. Potentially, a wheat sample, without
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54 drying, can be scanned for a few seconds on an NIR machine and from the spectra produce a very
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56 reasonable prediction of broiler performance, with only a small error associated with the equation
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(2.35% for gain:feed and 4.9% for live weight gain). The accuracy of all these predictions may even be improved further by eliminating outliers, which can justifiably be excluded and clearly seen from the actual versus predicted regression plots.

By including the Canadian wheat in the NIRS analysis of the dried and milled wheat samples the R^2_{cv} values were increased for most parameters and improvements observed in the R^2_{cv} values for TG (0.76), starch (0.79) and GE (0.86) are significant, in that, they are now greater than 0.75. A similar trend was observed when the Canadian wheat was included in the NIRS analysis of the undried and milled samples. Most parameters obtained increased R^2_{cv} values, with starch and GE having significant improvement, with small SECVs as a percentage of the mean (2.6 and 0.3 respectively). Therefore NIRS may also be an extremely useful tool for the determination of starch and gross energy content of a milled wheat sample. This could be an extremely beneficial finding, as the determination of these parameters by traditional methods can be costly and time consuming.

Conclusions

1. NIRS calibrations for milled wheat samples may be useful for determining specific weight, crude protein and rate of starch digestion.
2. NIRS calibrations for whole wheat samples (not dried) may be useful for determining wheat nutritive value.
3. Inclusion of the Canadian wheat samples to the NIRS analysis provides additional robust calibrations for gross energy and starch content of the milled wheat samples.

This study provides clear evidence that NIRS could be used as a rapid and accurate method for determining feed wheat quality, however, expansion of the dataset would be strongly recommended to further validate these findings.

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20 21 REFERENCES

- 22
23 Association of Official Analytical Chemists. (1990). *Official Methods of Analysis 15th ed.*,
24
25 Washington DC: AOAC.
26
27
28 Baker, C.W. and Barnes, R. (1990). The application of near infra-red spectroscopy to forage
29
30 evaluation in the Agricultural Development and Advisory Service. In: J. Wiseman and D.J.A.
31
32 Cole (Editors), *Feedstuff Evaluation*. Butterworths, London, pp. 337-354.
33
34
35 Barnes, R.J., Dhanoa, M.S. and Lister, S.J. (1989). Standard normal variate transformation and
36
37 de-trending of near infrared diffuse reflectance spectra. *Applied Spectroscopy*, **43**: 772-777.
38
39
40 Bedford, M.R. and Classen, H.L. (1993). An *in vitro* assay for prediction of broiler intestinal
41
42 viscosity and growth when fed rye-based diets in the presence of exogenous enzymes. *Poultry*
43
44 *Science*, **72**: 137-143.
45
46
47 Englyst, H.N., Quigley, M.E. and Hudson, G.J. (1994). Determination of dietary fibre as
48
49 nonstarch polysaccharides with gas-liquid-chromatographic, high-performance liquid-
50
51 chromatographic or spectrophotometric measurement of constituent sugars. *Analyst*, **119**: 1497-
52
53 1509.
54
55
56
57
58
59
60

1
2
3 Englyst, H.N., Veenstra, J. and Hudson, G.J. (1996). Measurement of rapidly available glucose
4 (RAG) in plant foods: a potential *in vitro* predictor of the glycaemic response. *British Journal of*
5
6 *Nutrition*, **75**: 327-337.
7
8

9
10 Garnsworthy, P.C., Wiseman, J. and Fegeros, K. (2000). Prediction of chemical, nutritive and
11
12 agronomic characteristics of wheat by near infrared spectroscopy. *Journal of Agricultural*
13
14 *Science, Cambridge*, **135**: 409-417.
15
16

17 Martens, H. and Naes, T. (1989). *Multivariate Calibration*. John Wiley and Sons, Chichester, pp
18
19 419.
20
21

22 McCleary, B.V., Gibson, T.S. and Mugford, D.C. (1997). Measurement of total starch in cereal
23
24 products by amyloglucosidase- α -amylase method: Collaborative Study. *Journal of the*
25
26 *Association of Official Analytical Chemists International*, **80**: 571-579.
27
28

29 McCracken, K.J. and Quintin, G. (2000). Metabolisable energy content of diets and broiler
30
31 performance as affected by wheat specific weight and enzyme supplementation. *British Poultry*
32
33 *Science*, **41**: 332-342.
34
35

36 McCracken, K.J., Preston, C.M. and Butler, C. (2002). Effects of wheat variety and specific
37
38 weight on dietary apparent metabolisable energy concentration and performance of broiler
39
40 chicks. *British Poultry Science*, **43**:253-260.
41
42

43 Miller, H.M., Wilkinson, J.M., McCracken, K.J., Knox, A., McNab, J. and Rose, S.P. (2001).
44
45 Nutritional value to farm livestock of wheat of low specific weight. HGCA Project Report No.
46
47 260, HGCA, London.
48
49

50 Wiseman, J. and Haresign, W. pp87-110. Nottingham: Nottingham University Press.
51

52 Osbourne, B.G., Fearn, T. and Hindle, P.H. (1993). *Practical NIR Spectroscopy with*
53
54 *Applications in Food and Beverage Analysis*. Harlow, Essex: Longman Scientific and Technical.
55
56
57
58
59
60

1
2
3 Park, R.S., Agnew, R.E., Gordon, F.J. and Steen, R.W.J. (1998). The use of near infrared
4 spectroscopy (NIRS) on undried samples of grass silage to predict chemical composition and
5 digestibility parameters. *Animal Feed Science and Technology*, **72**: 155-167.
6
7

8
9
10 Péron, A., Bastianelli, D., Oury, F.-X., Gomez, J. and Carré, B. (2005). Effects of food
11 deprivation and particle size of ground wheat on digestibility of food components in broilers fed
12 on a pelleted diet. *British Poultry Science*, **46**: 223-230.
13
14

15
16
17 Rose, S.P., Kettlewell, P.S., Reynolds, M.S. and Watts, M.R. (1993). The nutritive value of
18 different wheat varieties for poultry. *Proceedings of the Nutrition Society*, **52**: 206A.
19
20

21
22 Rose, S.P., Tucker, L.A., Kettlewell, P.S. and Collier, J.D.A. (2001). Rapid tests of wheat
23 nutritive value for growing chickens. *Journal of Cereal Science*, **34**: 181-190.
24
25

26
27 Scott, T.A., Silversides, F.G., Classen, H.L., Swift, M.L. and Bedford, M.R. (1998). Effect of
28 cultivar and environment on the feeding value of Western Canadian wheat and barley samples
29 with and without enzyme supplementation. *Canadian Journal of Animal Science*, **78**: 649-656.
30
31

32
33 Stoldt, W. (1952). Vorschlag zur Vereinheitlichung der Fettbestimmung in Lebensmitteln
34 (Suggestion to standardise the determination of fat in foodstuffs). *Fette, Seifen und*
35 *Anstrichmittel*, **54**: 206-207.
36
37

38
39
40 Van Soest, P.J. (1963). Use of detergents in the analysis of fibrous feeds. 1. Preparation of
41 fibre residues of low nitrogen contents. *Journal of the Association of Agricultural Chemists*, **46**:
42
43
44
45
46
47
48

49 Waldroup, P.W. (1997). Particle size reduction of cereal grains and its significance in poultry
50 nutrition. *Technical Bulletin PO 34-1997*. American Soybean Association, Singapore, pp14.
51
52

53 Weurding, R.E., Veldman, A., Veen, W.A.G., Van der Aar, P.J. and Verstegen, M.W.A. (2001).
54 Starch digestion rate in the small intestine of broiler chickens differs among feedstuffs. *Journal*
55 *of Nutrition*, **131**: 2329-2335.
56
57
58
59
60

1
2
3 Wiseman, J. (2000). Correlation between physical measurements and dietary energy values of
4 wheat for poultry and pigs. *Animal Feed Science and Technology*, **84**: 1-11.
5
6

7
8 Yun, S.H. and Matheson, N.K. (1990). Estimation of amylase content of starches after
9 precipitation of amylopectin by concanavalin-A. *Starch*, **42**: 302-305.
10
11
12
13
14
15
16
17
18
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Table 1. *Composition of diets*

Component	g/kg
Wheat	650
Hipro soya bean meal	200.5
Full fat soya bean	40
Fish meal	40
Soya bean/tallow blend	25
Limestone	8
Dicalcium phosphate	14
Trace minerals/ vitamins*	5
Sodium bicarbonate	2
Sodium chloride	2
Choline chloride	0.5
Lysine**	2.5
Methionine**	4.7
Threonine**	2.8
Maize starch**	3.0

*The trace mineral/vitamin mixture supplied (per kg feed): retinol 3.6 mg, cholecalciferol 0.125 mg, α -tocopherol 50 mg, thiamine 2 mg, riboflavin 7 mg, phylloquinone/menaquinone/menadione 3 mg, pyridoxine 5 mg, nicotinic acid 50 mg, calcium pantothenate 15 mg, folic acid 1 mg, biotin 0.2 mg, cobalamin 15 μ g, manganese 100 mg, iron 80 mg, zinc 80 mg, copper 10 mg, iodine 1 mg, cobalt 0.5 mg, selenium 0.2 mg, molybdenum 0.5 mg.

**For each wheat sample inclusions of lysine, methionine, threonine and maize starch were adjusted on the basis of the determined amino acid analysis of the wheat to equalise total concentrations across all diets.

Table 2. *Chemical and physical analysis of the wheat samples*

Parameter		Minimum	Maximum	Mean
Specific weight (kg/hl)		59	78	71
Thousand grain weight (g)		21.7	60.8	43.1
In vitro viscosity (cp)		3.2	44	12
N (g/kg DM)		12.5	32.7	20.2
NDF (g/kg DM)		101	195	141
Starch (g/kg DM)		547	719	633
Total NSP (g/kg DM)		81.7	138.8	107
Soluble NSP (g/kg DM)		8.4	38	23
GE (MJ/kg DM)		18.06	18.84	18.40
Amylose (g/kg DM)		115	211	159
Hardness ^a		8.4	66.7	42.1
Hardness ^b		2.9	74.1	36.0
RSD rate constant		1.33	4.35	2.50
Protein profile (%)	Band 1	2.1	7.9	5.0
	Band 2	9.1	18.8	14.5
	Band 3	10.2	23.6	18.4
	Band 4	24.3	48.1	35.4
	Band 5	20.9	37.4	26.6

^a = old SKCS equation ^b = new SKCS equation

Table 3. Range and standard deviation of all wheats (excluding the Canadian wheats)

Variable	Units	Mean	Min	Max	Std Dev	No of samples
Specific weight	kg/hl	70.72	59.00	78.00	4.03	138
Thousand grain weight	g	44.63	28.70	60.80	6.86	139
<i>In vitro</i> viscosity	cp	13.36	4.30	44.00	6.40	141
Nitrogen	g/kg DM	19.13	12.49	24.03	2.40	141
NDF	g/kg DM	138.87	101.30	178.60	12.72	141
Starch	g/kg DM	641.14	567.00	719.00	29.42	141
Total NSP	g/kg DM	106.96	81.70	138.80	11.24	141
Soluble NSP	g/kg DM	23.52	8.40	38.00	5.39	141
Lysine	g/kg DM	3.51	1.80	5.80	0.59	141
Threonine	g/kg DM	3.31	1.20	4.90	0.70	141
Gross Energy	MJ/kg DM	18.35	18.06	18.70	0.11	141
Amylose	g/kg DM	159.05	115.00	182.30	11.47	141
RSD (0.125h)	% starch	36.70	20.41	51.60	7.01	141
RSD (0.250h)	% starch	48.65	29.90	67.12	7.36	141
RSD (0.375h)	% starch	58.80	38.98	74.64	7.31	141
RSD (0.5h)	% starch	67.65	47.64	83.02	7.84	141
RSD (0.75h)	% starch	81.57	58.73	98.90	7.49	141
RSD (1h)	% starch	90.28	71.97	100.82	5.71	141
RSD (2h)	% starch	102.38	93.61	110.62	3.39	141
RSD Rate Constant	% degradation/h	2.58	1.34	4.35	0.60	141
Hardness	*	35.68	8.41	66.65	12.80	107
Protein profile (Band 1)	%	5.05	2.10	7.90	1.08	84
Protein profile (Band 2)	%	14.47	9.10	18.80	2.06	84
Protein profile (Band 3)	%	18.37	10.20	23.60	3.48	84
Protein profile (Band 4)	%	35.39	24.30	48.10	4.43	84
Protein profile (Band 5)	%	26.60	20.90	37.40	3.30	84
DMI (7-14d)	g/d	34.38	28.80	39.30	2.40	93
DMI (14-21d)	g/d	71.51	58.60	83.10	4.73	93
DMI (21-28d)	g/d	115.25	92.20	134.90	8.84	93
Total DMI	g/d	73.77	61.60	85.70	4.94	93
LWG (7-14d)	g/d	28.52	21.40	33.20	3.34	93
LWG (14-21d)	g/d	57.47	42.40	65.10	5.90	93
LWG (21-28d)	g/d	81.84	58.10	96.30	8.45	93
Total LWG	g/d	55.93	41.90	64.20	5.67	93
Gain:feed (7-14d)	*	82.75	73.10	90.60	5.06	93
Gain:feed (14-21d)	*	80.41	71.90	88.40	4.40	93
Gain:feed (21-28d)	*	71.11	61.50	78.20	3.20	93
Total gain:feed	*	75.79	67.20	81.70	3.59	93
<i>In vivo</i> viscosity	cp	5.89	3.31	12.98	1.97	93
ME:GE ratio	*	73.81	67.10	78.40	2.30	93
AME Content	MJ/kg DM	13.92	12.67	14.79	0.46	93
ME:Gain ratio	MJ/kg	18.31	16.72	20.86	0.90	93
DM Retention	%	72.13	69.70	75.30	1.31	61
Ileal DM Digestibility	%	69.98	62.70	75.60	2.66	61
Ileal Starch Digestibility	%	91.71	83.20	97.20	3.30	61
Ileal CP Digestibility	%	76.92	70.30	83.20	3.26	61

* = no units, R^2_{cv} = correlation coefficient of cross validation.

Table 4(a). *NIRS calibration statistics for chemical, physical and biological parameters for all dried milled wheat samples (excluding Canadian wheats)*

Variable	N	Mean	SEC	R ²	SECV	R ² _{cv}	Factors	SECV as % of mean
Specific weight	261	70.87	1.638	0.817	1.927	0.747	10	2.72
Thousand grain weight	272	44.81	3.314	0.754	3.997	0.643	10	8.92
<i>In vitro</i> viscosity	265	12.37	2.180	0.786	2.744	0.661	11	22.18
Nitrogen	272	19.12	0.249	0.989	0.312	0.983	11	1.63
NDF	277	138.81	7.797	0.600	8.825	0.495	8	6.36
Starch	273	640.69	13.642	0.778	15.555	0.711	9	2.43
Total NSP	274	106.60	5.157	0.768	6.010	0.685	9	5.64
Soluble NSP	267	23.72	3.049	0.622	3.572	0.480	9	15.06
Lysine	268	3.48	0.298	0.656	0.333	0.575	8	9.56
Threonine	266	3.38	0.291	0.765	0.312	0.731	8	9.24
Gross Energy	274	18.36	0.045	0.818	0.052	0.760	8	0.28
Amylose	268	160.44	4.983	0.735	5.863	0.632	10	3.65
RSD (0.125h)	274	36.47	2.717	0.840	2.972	0.808	8	8.15
RSD (0.250h)	276	48.49	2.590	0.872	3.233	0.800	10	6.67
RSD (0.375h)	272	58.79	2.634	0.867	3.235	0.799	11	5.50
RSD (0.5h)	277	67.65	3.163	0.834	3.704	0.771	9	5.48
RSD (0.75h)	275	81.52	3.021	0.831	3.422	0.782	9	4.20
RSD (1h)	281	90.26	2.376	0.826	2.911	0.739	10	3.22
RSD (2h)	278	102.43	1.768	0.724	2.047	0.630	10	2.00
RSD Rate Constant	272	2.55	0.234	0.826	0.263	0.780	9	10.33
Hardness	204	35.72	4.530	0.865	5.592	0.794	9	15.66
Protein profile (Band 1)	165	5.05	0.447	0.831	0.546	0.749	10	10.81
Protein profile (Band 2)	161	14.42	0.727	0.867	0.944	0.777	10	6.55
Protein profile (Band 3)	166	18.33	1.714	0.755	2.145	0.618	9	11.70
Protein profile (Band 4)	164	35.41	1.549	0.879	2.135	0.771	10	6.03
Protein profile (Band 5)	167	26.56	1.880	0.667	2.021	0.613	6	7.61
DMI (7-14d)	182	34.37	1.306	0.704	1.616	0.546	9	4.70
DMI (14-21d)	179	71.43	2.550	0.699	2.932	0.600	8	4.10
DMI (21-28d)	177	115.20	3.964	0.794	4.937	0.680	9	4.29
Total DMI	176	73.92	1.917	0.841	2.609	0.705	10	3.53
LWG (7-14d)	178	28.49	1.519	0.788	1.863	0.680	9	6.54
LWG (14-21d)	178	57.44	2.718	0.785	3.442	0.654	9	5.99
LWG (21-28d)	172	82.31	3.068	0.839	4.058	0.720	10	4.93
Total LWG	175	55.90	2.398	0.816	2.933	0.723	9	5.25
Gain:feed (7-14d)	182	82.63	2.641	0.724	3.433	0.531	9	4.15
Gain:feed (14-21d)	185	80.39	2.411	0.699	2.949	0.549	9	3.67
Gain:feed (21-28d)	181	71.27	2.018	0.526	2.384	0.344	8	3.35
Total gain:feed	184	75.81	1.987	0.683	2.603	0.456	10	3.43
<i>In vivo</i> viscosity	172	5.53	0.909	0.507	1.096	0.303	6	19.84
ME:GE	178	73.74	1.025	0.787	1.249	0.683	8	1.69
AME Content	182	13.92	0.229	0.723	0.272	0.608	8	1.95
ME:Gain	168	18.28	0.285	0.879	0.389	0.775	10	2.13
DM Retention	122	72.13	1.067	0.334	1.124	0.264	4	1.56
Ileal DM Digestibility	118	70.03	1.900	0.407	1.957	0.376	3	2.79
Ileal Starch Digestibility	117	91.94	1.789	0.647	2.158	0.506	6	2.35
Ileal CP Digestibility	118	77.03	2.269	0.476	2.370	0.427	4	3.08

N = number of spectra in the calibration equation, SEC = standard error of calibration, R² = coefficient of determination of the calibration, SECV = standard error of cross validation, R²_{cv} = correlation coefficient of cross validation, factors = number of actual terms used to estimate the parameter.

Table 4(b). *NIRS sub-calibration and validation statistics for chemical, physical and biological parameters of dried milled wheat (excluding Canadian wheats)*

Variable	N	Mean _{cal}	SEC	R ² _{cal}	Mean _{val}	SEP	R ² _{val}	SEP as % of Mean _{val}
Specific weight	206	70.79	1.494	0.846	71.02	2.605	0.619	3.668
Thousand grain weight	211	45.14	3.025	0.785	44.18	4.794	0.633	10.852
<i>In vitro</i> viscosity	209	12.43	2.279	0.770	13.68	6.692	0.262	48.905
Nitrogen	213	19.07	0.257	0.990	19.31	0.649	0.906	3.360
NDF	220	138.30	6.745	0.749	140.01	10.274	0.171	7.338
Starch	220	641.37	13.229	0.769	639.41	23.012	0.597	3.599
Total NSP	220	107.10	5.141	0.776	106.71	6.437	0.713	6.032
Soluble NSP	216	23.72	3.034	0.642	23.26	4.012	0.512	17.249
Lysine	215	3.50	0.275	0.733	3.57	0.455	0.525	12.743
Threonine	209	3.37	0.251	0.820	3.38	0.418	0.697	12.390
Gross Energy	221	18.36	0.051	0.772	18.36	0.041	0.824	0.224
Amylose	213	160.51	4.916	0.745	158.26	7.626	0.617	4.819
RSD (0.125h)	211	36.17	1.982	0.915	38.09	3.921	0.752	10.296
RSD (0.250h)	219	47.96	2.248	0.901	50.38	4.410	0.697	8.754
RSD (0.375h)	220	58.14	2.759	0.853	60.53	4.270	0.698	7.054
RSD (0.5h)	218	67.25	2.657	0.885	68.78	4.660	0.614	6.775
RSD (0.75h)	217	81.49	2.657	0.876	82.57	4.335	0.626	5.251
RSD (1h)	224	90.01	2.373	0.830	91.31	3.295	0.671	3.609
RSD (2h)	219	102.24	1.455	0.806	103.11	2.449	0.497	2.375
RSD Rate Constant	208	2.50	0.164	0.911	2.70	0.348	0.745	12.904
Hardness	160	36.63	4.132	0.891	34.45	9.812	0.481	28.482
Protein profile (Band 1)	136	4.97	0.438	0.818	5.39	0.624	0.752	11.577
Protein profile (Band 2)	132	14.57	0.787	0.867	14.11	1.202	0.544	8.516
Protein profile (Band 3)	133	18.25	1.308	0.860	18.86	2.305	0.476	12.222
Protein profile (Band 4)	128	35.27	1.135	0.935	35.37	2.412	0.766	6.819
Protein profile (Band 5)	132	26.66	1.193	0.887	26.15	1.797	0.371	6.874
DMI (7-14d)	151	34.48	1.373	0.644	34.04	2.220	0.407	6.523
DMI (14-21d)	148	71.50	2.402	0.700	71.36	4.898	0.349	6.864
DMI (21-28d)	146	114.74	3.559	0.834	116.79	7.446	0.368	6.375
Total DMI	149	73.66	2.164	0.792	74.14	4.598	0.377	6.202
LWG (7-14d)	148	28.44	1.378	0.824	28.41	2.517	0.584	8.862
LWG (14-21d)	145	57.30	2.160	0.860	57.92	4.182	0.621	7.219
LWG (21-28d)	144	81.57	3.006	0.852	82.96	5.883	0.531	7.092
Total LWG	147	55.62	2.222	0.841	56.41	4.613	0.406	8.177
Gain:feed (7-14d)	150	82.75	2.543	0.751	82.38	3.546	0.584	4.304
Gain:feed (14-21d)	150	80.18	2.119	0.775	81.15	2.729	0.519	3.363
Gain:feed (21-28d)	148	71.16	1.873	0.599	71.14	3.181	0.118	4.471
Total gain:feed	150	75.67	1.859	0.738	76.06	2.736	0.325	3.598
<i>In vivo</i> viscosity	142	5.73	0.927	0.696	5.36	1.014	0.124	18.911
ME:GE	149	73.93	1.143	0.715	73.30	1.69	0.61	2.31
AME Content	145	13.93	0.166	0.848	13.84	0.33	0.56	2.38
ME:Gain	145	18.30	0.354	0.809	18.11	0.72	0.42	3.97
DM Retention	102	72.21	1.120	0.292	71.75	1.330	0.009	1.853
Ileal DM Digestibility	102	69.97	2.167	0.374	69.99	2.023	0.330	2.890
Ileal Starch Digestibility	96	92.52	1.809	0.467	89.74	4.298	0.619	4.790
Ileal CP Digestibility	100	76.75	2.428	0.487	77.84	2.631	0.181	3.381

N = number of spectra in the calibration equation, Mean_{cal} = mean of calibration dataset, SEC = standard error of calibration, R²_{cal} = coefficient of determination of the calibration, SEP = standard error of prediction, R²_{val} = correlation coefficient of the validation, Mean_{val} = mean of independent validation set.

Table 5(a). *NIRS calibration statistics for chemical, physical and biological parameters for all undried milled wheat samples (excluding Canadian wheats)*

Variable	N	Mean	SEC	R ²	SECV	R ² _{cv}	Factors	SECV as % of mean
Specific weight	265	70.75	1.802	0.798	2.213	0.697	10	3.13
Thousand grain weight	275	44.65	3.272	0.770	4.192	0.624	10	9.39
<i>In vitro</i> viscosity	263	12.27	2.314	0.745	2.888	0.602	9	23.54
Nitrogen	267	19.10	0.252	0.989	0.315	0.983	10	1.65
NDF	273	138.98	7.011	0.670	8.773	0.494	10	6.31
Starch	271	641.09	13.855	0.773	17.050	0.655	10	2.66
Total NSP	275	106.74	5.700	0.724	6.110	0.683	8	5.72
Soluble NSP	271	23.68	4.032	0.354	4.069	0.342	2	17.19
Lysine	267	3.45	0.326	0.438	0.341	0.392	4	9.89
Threonine	269	3.30	0.300	0.800	0.383	0.675	10	11.60
Gross Energy	274	18.35	0.038	0.856	0.052	0.739	11	0.28
Amylose	268	160.15	6.152	0.600	6.638	0.533	7	4.14
RSD (0.125h)	273	36.67	2.501	0.871	2.883	0.828	8	7.86
RSD (0.250h)	268	48.36	2.726	0.855	2.958	0.829	7	6.12
RSD (0.375h)	269	58.57	3.239	0.788	3.345	0.774	5	5.71
RSD (0.5h)	273	67.58	3.051	0.842	3.552	0.786	8	5.26
RSD (0.75h)	271	81.70	3.117	0.804	3.449	0.760	7	4.22
RSD (1h)	278	90.27	2.592	0.783	3.046	0.699	8	3.37
RSD (2h)	268	102.54	1.820	0.694	1.991	0.634	8	1.94
RSD Rate Constant	270	2.55	0.246	0.807	0.252	0.797	5	9.89
Hardness	205	36.07	6.366	0.735	6.584	0.716	5	18.25
Protein profile (Band 1)	167	5.04	0.439	0.835	0.663	0.625	10	13.15
Protein profile (Band 2)	164	14.48	0.963	0.780	1.164	0.680	8	8.04
Protein profile (Band 3)	166	18.36	2.045	0.653	2.150	0.618	6	11.71
Protein profile (Band 4)	156	35.39	1.217	0.917	1.579	0.860	10	4.46
Protein profile (Band 5)	164	26.57	1.271	0.850	1.848	0.682	10	6.95
DMI (7-14d)	183	34.40	1.029	0.817	1.408	0.657	9	4.09
DMI (14-21d)	180	71.52	2.347	0.741	2.810	0.627	9	3.93
DMI (21-28d)	177	115.49	4.308	0.740	5.118	0.632	8	4.43
Total DMI	181	73.89	2.421	0.752	2.878	0.647	8	3.89
LWG (7-14d)	178	28.64	1.189	0.864	1.607	0.751	10	5.61
LWG (14-21d)	175	58.02	2.279	0.832	2.860	0.734	9	4.93
LWG (21-28d)	175	82.31	3.294	0.819	4.382	0.678	10	5.32
Total LWG	177	56.31	2.157	0.838	2.750	0.736	9	4.88
Gain:feed (7-14d)	178	83.10	2.508	0.734	2.991	0.619	7	3.60
Gain:feed (14-21d)	178	80.52	1.870	0.813	2.552	0.650	10	3.17
Gain:feed (21-28d)	180	71.22	2.290	0.361	2.360	0.325	4	3.31
Total gain:feed	177	75.87	1.418	0.838	2.036	0.665	11	2.68
<i>In vivo</i> viscosity	180	5.77	1.190	0.537	1.361	0.402	7	23.57
ME:GE	179	73.80	1.117	0.746	1.339	0.634	8	1.81
AME Content	182	13.92	0.230	0.715	0.273	0.598	8	1.96
ME:Gain	173	18.26	0.341	0.818	0.441	0.696	9	2.42
DM Retention	118	72.05	0.913	0.458	1.068	0.267	6	1.48
Ileal DM Digestibility	120	70.10	1.559	0.609	2.215	0.222	8	3.16
Ileal Starch Digestibility	119	91.90	2.162	0.517	2.321	0.460	4	2.53
Ileal CP Digestibility	122	76.92	2.840	0.233	2.907	0.193	2	3.78

N = number of spectra in the calibration equation, SEC = standard error of calibration,

R² = coefficient of determination of the calibration, SECV = standard error of cross validation,

R²_{cv} = correlation coefficient of cross validation, factors = number of terms used to estimate the parameter.

Table 5(b). *NIRS sub-calibration and validation statistics for chemical, physical and biological parameters of undried milled wheat (excluding Canadian wheats)*

Variable	N	Mean _{cal}	SEC	R ² _{cal}	Mean _{val}	SEP	R ² _{val}	SEP as % of Mean _{val}
Specific weight	215	70.70	1.492	0.850	71.02	2.853	0.517	4.017
Thousand grain weight	217	44.82	3.308	0.762	44.18	4.791	0.628	10.845
<i>In vitro</i> viscosity	206	12.22	2.237	0.757	13.68	6.179	0.458	45.162
Nitrogen	216	19.09	0.318	0.984	19.31	0.707	0.888	3.661
NDF	215	138.39	6.976	0.720	140.01	10.644	0.194	7.602
Starch	214	642.04	12.361	0.785	639.41	27.124	0.411	4.242
Total NSP	218	106.75	5.447	0.737	106.71	6.587	0.682	6.172
Soluble NSP	217	23.66	4.240	0.321	23.26	4.366	0.411	18.773
Lysine	212	3.44	0.323	0.419	3.57	0.511	0.476	14.318
Threonine	220	3.31	0.338	0.748	3.38	0.556	0.458	16.478
Gross Energy	216	18.35	0.044	0.810	18.36	0.051	0.734	0.276
Amylose	212	160.72	5.989	0.622	158.26	8.313	0.491	5.253
RSD (0.125h)	211	36.11	2.540	0.861	38.09	3.936	0.741	10.335
RSD (0.250h)	214	48.06	2.264	0.905	50.38	5.233	0.595	10.387
RSD (0.375h)	213	58.08	3.070	0.806	60.53	4.356	0.685	7.196
RSD (0.5h)	213	67.26	3.008	0.852	68.78	4.383	0.663	6.372
RSD (0.75h)	211	81.57	2.563	0.876	82.57	4.352	0.605	5.271
RSD (1h)	216	90.12	2.237	0.834	91.31	3.530	0.602	3.866
RSD (2h)	214	102.39	1.726	0.727	103.11	2.607	0.433	2.528
RSD Rate Constant	208	2.50	0.157	0.915	2.70	0.349	0.745	12.933
Hardness	161	36.59	4.410	0.875	34.45	11.212	0.358	32.544
Protein profile (Band 1)	136	4.97	0.361	0.876	5.39	0.851	0.548	15.782
Protein profile (Band 2)	127	14.51	0.691	0.904	14.11	1.948	0.293	13.800
Protein profile (Band 3)	136	18.26	1.948	0.694	18.86	2.737	0.289	14.515
Protein profile (Band 4)	131	35.34	1.078	0.943	35.37	2.782	0.627	7.865
Protein profile (Band 5)	130	26.73	1.046	0.916	26.15	2.268	0.240	8.674
DMI (7-14d)	148	34.55	1.399	0.621	34.04	1.906	0.557	5.601
DMI (14-21d)	146	71.61	2.455	0.663	71.36	3.762	0.611	5.272
DMI (21-28d)	145	114.97	4.080	0.762	116.79	7.436	0.445	6.367
Total DMI	150	73.75	2.461	0.729	74.14	4.042	0.527	5.452
LWG (7-14d)	152	28.55	1.383	0.825	28.41	1.753	0.786	6.172
LWG (14-21d)	146	57.69	1.839	0.892	57.92	3.611	0.685	6.233
LWG (21-28d)	144	82.44	3.356	0.810	82.96	6.226	0.493	7.504
Total LWG	148	56.04	2.300	0.826	56.41	3.580	0.660	6.346
Gain:feed (7-14d)	152	82.84	2.298	0.799	82.38	3.399	0.615	4.126
Gain:feed (14-21d)	152	80.24	1.912	0.817	81.15	3.199	0.512	3.942
Gain:feed (21-28d)	144	71.29	1.628	0.655	71.14	2.781	0.349	3.910
Total gain:feed	146	75.77	1.401	0.850	76.06	2.910	0.399	3.826
<i>In vivo</i> viscosity	137	5.61	1.160	0.370	5.36	0.878	0.230	16.360
ME:GE	147	73.95	1.047	0.752	73.30	1.74	0.57	2.38
AME Content	149	13.94	0.266	0.605	13.84	0.41	0.32	2.95
ME:Gain	144	18.28	0.342	0.815	18.11	0.77	0.39	4.26
DM Retention	102	72.21	0.870	0.573	71.75	1.300	0.230	1.811
Ileal DM Digestibility	100	70.12	2.410	0.115	69.99	1.860	0.238	2.657
Ileal Starch Digestibility	100	92.24	1.863	0.552	89.74	3.836	0.612	4.275
Ileal CP Digestibility	102	76.74	2.957	0.259	77.84	2.171	0.275	2.789

N = number of spectra in the calibration equation, Mean_{cal} = mean of calibration dataset, SEC = standard error of calibration, R²_{cal} = coefficient of determination of the calibration, SEP = standard error of prediction, R²_{val} = correlation coefficient of the validation, Mean_{val} = mean of independent validation set.

Table 6(a). *NIRS calibration statistics for chemical, physical and biological parameters for all dried whole kernel wheat samples (excluding Canadian wheats)*

Variable	N	Mean	SEC	R ²	SECV	R ² _{cv}	Factors	SECV as % of mean
Specific weight	208	71.02	1.606	0.783	1.847	0.720	9	2.60
Thousand grain weight	206	43.98	2.983	0.739	3.280	0.686	9	7.46
<i>In vitro</i> viscosity	206	12.50	2.487	0.782	3.121	0.655	11	24.98
Nitrogen	207	18.85	0.641	0.922	0.732	0.898	8	3.88
NDF	216	140.89	7.359	0.643	8.365	0.540	8	5.94
Starch	213	631.53	13.281	0.712	14.761	0.643	8	2.34
Total NSP	208	104.20	4.883	0.730	5.714	0.629	10	5.48
Soluble NSP	208	22.70	3.970	0.156	3.996	0.141	2	17.61
Lysine	203	3.52	0.307	0.637	0.357	0.512	10	10.16
Threonine	208	3.17	0.354	0.631	0.421	0.478	10	13.29
Gross Energy	204	18.34	0.049	0.741	0.058	0.649	10	0.32
Amylose	208	158.80	6.683	0.614	7.306	0.539	7	4.60
RSD (0.125h)	216	36.13	4.071	0.657	4.849	0.516	10	13.42
RSD (0.250h)	215	47.83	4.159	0.678	4.844	0.565	11	10.13
RSD (0.375h)	213	57.76	4.086	0.677	4.915	0.533	11	8.51
RSD (0.5h)	209	66.60	4.067	0.724	4.711	0.630	10	7.07
RSD (0.75h)	213	80.53	3.956	0.709	4.432	0.636	9	5.50
RSD (1h)	212	89.02	3.099	0.685	3.520	0.595	8	3.95
RSD (2h)	214	102.61	2.210	0.592	2.665	0.413	9	2.60
RSD Rate Constant	208	2.47	0.283	0.726	0.350	0.584	11	14.19
Hardness	210	35.47	7.383	0.664	8.046	0.601	8	22.68
Protein profile (Band 1)	99	5.16	0.377	0.880	0.544	0.752	11	10.53
Protein profile (Band 2)	104	15.57	1.290	0.186	1.330	0.140	3	8.54
Protein profile (Band 3)	101	18.62	1.333	0.815	1.582	0.738	8	8.50
Protein profile (Band 4)	101	33.39	1.776	0.710	1.830	0.690	5	5.48
Protein profile (Band 5)	99	26.98	1.517	0.750	1.793	0.649	8	6.64
DMI (7-14d)	120	33.50	1.524	0.616	1.609	0.572	4	4.80
DMI (14-21d)	115	69.84	2.159	0.770	2.850	0.597	10	4.08
DMI (21-28d)	116	112.97	3.348	0.867	4.695	0.738	11	4.16
Total DMI	115	72.12	1.794	0.866	2.444	0.749	11	3.39
LWG (7-14d)	118	27.50	1.944	0.723	2.020	0.700	4	7.35
LWG (14-21d)	120	55.99	3.849	0.673	4.003	0.645	4	7.15
LWG (21-28d)	118	80.07	4.537	0.784	4.990	0.738	6	6.23
Total LWG	117	54.50	2.684	0.827	3.052	0.776	7	5.60
Gain:feed (7-14d)	122	82.02	3.566	0.628	3.604	0.618	3	4.39
Gain:feed (14-21d)	116	80.23	1.688	0.896	1.903	0.868	7	2.37
Gain:feed (21-28d)	112	71.86	1.950	0.570	2.022	0.551	1	2.81
Total gain:feed	119	75.58	2.065	0.764	2.164	0.741	4	2.86
<i>In vivo</i> viscosity	121	6.45	1.499	0.469	1.664	0.362	6	25.79
ME:GE	120	75.03	0.947	0.501	1.145	0.265	8	1.53
AME Content	118	14.16	0.227	0.348	0.231	0.320	3	1.63
ME:Gain	112	18.63	0.475	0.674	0.487	0.659	4	2.61
DM Retention	122	72.13	1.148	0.229	1.203	0.148	4	1.67
Ileal DM Digestibility	122	69.98	1.669	0.603	2.066	0.390	9	2.95
Ileal Starch Digestibility	117	91.94	1.981	0.582	2.201	0.483	6	2.39
Ileal CP Digestibility	119	76.83	1.583	0.759	1.988	0.617	9	2.59

N = number of spectra in the calibration equation, SEC = standard error of calibration,

R² = coefficient of determination of the calibration, SECV = standard error of cross validation,

R²_{cv} = correlation coefficient of cross validation, factors = number of actual terms used to estimate the parameter.

Table 6(b). *NIRS sub-calibration and validation statistics for chemical, physical and biological parameters of dried whole kernel wheat (excluding Canadian wheats)*

Variable	N	Mean _{cal}	SEC	R ²	Mean _{val}	SEP	R ² _{val}	SEP as % of Mean _{val}
Specific weight	160	70.85	1.240	0.874	71.76	2.245	0.596	3.128
Thousand grain weight	166	44.10	2.545	0.822	43.83	4.331	0.493	9.882
<i>In vitro</i> viscosity	163	12.25	2.343	0.753	13.60	5.119	0.590	37.629
Nitrogen	162	18.95	0.530	0.944	18.92	0.894	0.851	4.728
NDF	168	141.44	7.224	0.641	138.72	8.200	0.551	5.912
Starch	169	630.60	11.774	0.764	635.09	20.048	0.490	3.157
Total NSP	164	104.74	3.932	0.813	103.05	8.460	0.366	8.210
Soluble NSP	165	23.01	3.646	0.291	21.63	4.812	0.067	22.245
Lysine	162	3.51	0.345	0.540	3.49	0.665	0.060	19.051
Threonine	163	3.15	0.305	0.730	3.19	0.487	0.450	15.283
Gross Energy	162	18.34	0.051	0.712	18.35	0.079	0.550	0.432
Amylose	163	158.26	6.064	0.699	159.45	9.144	0.239	5.735
RSD (0.125h)	172	36.09	5.039	0.472	36.31	5.332	0.511	14.687
RSD (0.250h)	172	47.80	4.814	0.569	48.00	6.377	0.462	13.285
RSD (0.375h)	169	57.83	4.933	0.529	57.99	6.063	0.450	10.455
RSD (0.5h)	166	66.75	3.836	0.761	66.42	5.567	0.542	8.382
RSD (0.75h)	167	80.64	3.973	0.707	80.40	6.605	0.423	8.215
RSD (1h)	169	89.06	3.029	0.695	89.38	4.165	0.588	4.660
RSD (2h)	167	102.62	1.725	0.767	102.51	2.702	0.391	2.636
RSD Rate Constant	167	2.50	0.337	0.634	2.50	0.488	0.482	19.516
Hardness	167	36.01	6.738	0.716	35.32	10.657	0.385	30.168
Protein profile (Band 1)	81	5.13	0.360	0.905	5.46	0.882	0.239	16.150
Protein profile (Band 2)	80	15.45	1.021	0.373	16.01	1.684	0.008	10.520
Protein profile (Band 3)	78	18.68	1.032	0.890	18.49	2.823	0.516	15.268
Protein profile (Band 4)	84	33.31	1.143	0.878	33.82	3.930	0.147	11.622
Protein profile (Band 5)	81	27.17	1.719	0.629	26.10	2.830	0.391	10.844
DMI (7-14d)	93	33.20	1.290	0.728	34.32	2.323	0.294	6.769
DMI (14-21d)	94	69.47	3.117	0.496	70.57	4.027	0.409	5.706
DMI (21-28d)	93	112.34	4.737	0.705	113.38	8.515	0.476	7.510
Total DMI	96	71.98	3.126	0.601	72.85	3.986	0.523	5.471
LWG (7-14d)	93	27.27	1.244	0.880	28.26	2.882	0.572	10.197
LWG (14-21d)	94	55.65	3.866	0.648	56.67	4.266	0.660	7.529
LWG (21-28d)	91	79.94	4.041	0.824	80.32	7.256	0.559	9.034
Total LWG	95	54.68	2.485	0.850	55.08	3.965	0.673	7.197
Gain:feed (7-14d)	95	81.88	2.324	0.833	82.26	4.657	0.528	5.661
Gain:feed (14-21d)	92	80.18	1.680	0.901	80.21	1.758	0.877	2.192
Gain:feed (21-28d)	93	71.69	1.527	0.806	70.92	3.654	0.170	5.151
Total gain:feed	93	75.83	1.345	0.895	75.50	3.475	0.527	4.603
<i>In vivo</i> viscosity	96	6.57	1.472	0.522	6.00	2.044	0.232	34.049
ME:GE	94	75.01	0.878	0.509	75.08	1.45	0.19	1.93
AME Content	94	14.15	0.220	0.328	14.13	0.31	0.41	2.17
ME:Gain	92	18.70	0.595	0.554	18.56	0.69	0.49	3.74
DM Retention	96	72.12	0.929	0.411	72.20	1.494	0.197	2.069
Ileal DM Digestibility	96	70.06	1.622	0.582	69.66	2.024	0.607	2.905
Ileal Starch Digestibility	96	91.48	1.687	0.740	92.55	3.313	0.323	3.580
Ileal CP Digestibility	96	77.19	1.957	0.604	75.94	2.816	0.369	3.708

N = number of spectra in the calibration equation, Mean_{cal} = mean of calibration dataset, SEC = standard error of calibration, R² = coefficient of determination of the calibration, SEP = standard error of prediction, R²_{val} = correlation coefficient of the validation, Mean_{val} = mean of independent validation set.

Table 7(a). *NIRS calibration statistics for chemical, physical and biological parameters for all undried whole kernel wheats (excluding Canadian wheats)*

Variable	N	Mean	SEC	R ²	SECV	R ² _{cv}	Factors	SECV as % of mean
Specific weight	180	71.66	1.235	0.806	1.528	0.703	10	2.13
Thousand grain weight	186	44.27	2.834	0.785	3.380	0.695	11	7.63
<i>In vitro</i> viscosity	183	12.43	2.385	0.808	2.899	0.717	10	23.33
Nitrogen	186	18.86	0.663	0.918	0.751	0.896	7	3.98
NDF	193	141.82	8.254	0.527	8.735	0.473	6	6.16
Starch	189	630.04	13.416	0.702	13.987	0.675	6	2.22
Total NSP	187	103.71	5.648	0.641	5.950	0.599	6	5.74
Soluble NSP	190	22.52	4.238	0.157	4.279	0.138	1	19.00
Lysine	185	3.56	0.278	0.778	0.344	0.660	10	9.66
Threonine	187	3.13	0.417	0.577	0.473	0.453	8	15.10
Gross Energy	184	18.34	0.054	0.707	0.062	0.618	7	0.34
Amylose	189	158.51	7.010	0.569	7.246	0.539	5	4.57
RSD (0.125h)	196	35.61	5.126	0.445	5.507	0.370	5	15.47
RSD (0.250h)	194	47.53	5.508	0.430	5.686	0.402	4	11.96
RSD (0.375h)	192	57.42	5.418	0.428	5.622	0.390	4	9.79
RSD (0.5h)	194	65.79	5.260	0.520	5.909	0.400	7	8.98
RSD (0.75h)	194	79.47	4.752	0.536	5.247	0.439	6	6.60
RSD (1h)	194	88.34	3.580	0.525	3.916	0.435	6	4.43
RSD (2h)	193	102.76	2.083	0.607	2.666	0.368	10	2.59
RSD Rate Constant	189	2.42	0.397	0.429	0.419	0.371	4	17.31
Hardness	189	34.40	8.401	0.523	8.940	0.462	6	25.99
Protein profile (Band 1)	104	5.19	0.450	0.834	0.580	0.725	9	11.19
Protein profile (Band 2)	104	15.57	1.325	0.142	1.343	0.122	1	8.62
Protein profile (Band 3)	104	18.59	1.879	0.641	2.025	0.582	4	10.90
Protein profile (Band 4)	102	33.36	1.804	0.700	1.889	0.668	4	5.66
Protein profile (Band 5)	104	27.12	2.179	0.510	2.399	0.404	5	8.85
DMI (7-14d)	118	33.49	1.284	0.725	1.460	0.645	6	4.36
DMI (14-21d)	118	69.96	3.261	0.472	3.279	0.464	2	4.69
DMI (21-28d)	118	112.35	3.703	0.833	4.561	0.746	10	4.06
Total DMI	121	72.11	2.790	0.694	2.985	0.647	6	4.14
LWG (7-14d)	118	27.56	1.636	0.804	1.792	0.763	6	6.50
LWG (14-21d)	116	56.01	2.728	0.823	3.030	0.780	6	5.41
LWG (21-28d)	120	80.28	3.926	0.840	4.737	0.767	9	5.90
Total LWG	118	54.75	2.253	0.873	2.698	0.817	8	4.93
Gain:feed (7-14d)	118	81.88	2.529	0.816	2.870	0.761	7	3.51
Gain:feed (14-21d)	118	80.04	1.948	0.865	2.315	0.810	8	2.89
Gain:feed (21-28d)	115	71.35	1.942	0.717	2.009	0.703	5	2.82
Total gain:feed	115	75.69	1.554	0.866	1.777	0.825	7	2.35
<i>In vivo</i> viscosity	117	6.43	0.928	0.781	1.371	0.537	11	21.34
ME:GE	122	75.08	0.905	0.586	1.186	0.274	8	1.58
AME Content	118	14.14	0.218	0.729	0.221	0.420	12	1.56
ME:Gain	112	18.61	0.344	0.836	0.472	0.690	11	2.54
DM Retention	122	72.13	0.850	0.578	1.132	0.246	9	1.57
Ileal DM Digestibility	120	70.10	2.005	0.353	2.214	0.207	5	3.16
Ileal Starch Digestibility	117	91.92	1.804	0.662	2.091	0.545	7	2.27
Ileal CP Digestibility	118	77.12	2.038	0.571	2.219	0.491	6	2.88

N = number of spectra in the calibration equation, SEC = standard error of calibration,

R² = coefficient of determination of the calibration, SECV = standard error of cross validation,

R²_{cv} = correlation coefficient of cross validation, factors = number of actual terms used to estimate the parameter.

Table 7(b). *NIRS sub-calibration and validation statistics for chemical, physical and biological parameters of undried whole kernel wheat (excluding Canadian wheats)*

Variable	N	Mean _{cal}	SEC	R ²	Mean _{val}	SEP	R ² _{val}	SEP as % of Mean _{val}
Specific weight	146	71.34	1.299	0.819	72.21	2.237	0.414	3.098
Thousand grain weight	148	44.32	2.903	0.784	44.05	3.949	0.602	8.966
<i>In vitro</i> viscosity	145	12.40	2.152	0.812	13.21	4.832	0.602	36.580
Nitrogen	146	18.74	0.481	0.960	18.95	1.026	0.819	5.413
NDF	156	142.75	8.925	0.447	139.54	8.823	0.517	6.323
Starch	154	630.44	10.621	0.818	633.80	20.083	0.461	3.169
Total NSP	152	104.45	5.359	0.677	102.69	7.342	0.466	7.150
Soluble NSP	150	22.78	3.687	0.343	21.58	5.232	0.042	24.240
Lysine	148	3.55	0.277	0.787	3.51	0.664	0.159	18.910
Threonine	150	3.13	0.403	0.577	3.19	0.566	0.367	17.714
Gross Energy	146	18.34	0.055	0.686	18.36	0.083	0.546	0.452
Amylose	149	158.04	6.931	0.641	159.13	7.393	0.292	4.646
RSD (0.125h)	156	35.67	4.869	0.494	35.36	5.994	0.325	16.950
RSD (0.250h)	156	47.43	5.292	0.480	47.32	6.496	0.302	13.728
RSD (0.375h)	154	57.31	5.365	0.440	57.31	5.915	0.390	10.321
RSD (0.5h)	155	65.94	5.480	0.503	65.59	6.507	0.274	9.922
RSD (1h)	156	79.64	4.801	0.551	79.79	6.946	0.254	8.705
RSD (0.75h)	156	88.33	3.654	0.512	88.80	4.653	0.325	5.239
RSD (2h)	153	102.92	2.584	0.442	102.34	2.490	0.314	2.433
RSD Rate Constant	155	2.44	0.390	0.475	2.44	0.510	0.302	20.880
Hardness	152	34.92	5.979	0.757	34.38	10.788	0.414	31.376
Protein profile (Band 1)	83	5.11	0.308	0.929	5.46	0.962	0.266	17.627
Protein profile (Band 2)	84	15.47	1.193	0.247	16.01	1.815	0.007	11.339
Protein profile (Band 3)	84	18.61	1.607	0.740	18.49	2.819	0.396	15.245
Protein profile (Band 4)	81	33.60	1.615	0.698	33.82	2.587	0.472	7.650
Protein profile (Band 5)	84	27.36	2.266	0.410	26.10	2.744	0.431	10.515
DMI (7-14d)	91	33.40	1.132	0.792	34.32	2.444	0.153	7.121
DMI (14-21d)	96	69.69	3.378	0.456	70.57	4.637	0.224	6.571
DMI (21-28d)	94	112.44	3.490	0.840	113.38	8.932	0.383	7.878
Total DMI	92	71.83	2.022	0.828	72.85	4.014	0.502	5.510
LWG (7-14d)	94	27.33	1.592	0.807	28.26	2.283	0.661	8.077
LWG (14-21d)	94	55.65	3.098	0.774	56.67	4.349	0.625	7.675
LWG (21-28d)	93	80.39	4.026	0.825	80.32	7.216	0.526	8.984
Total LWG	94	54.39	2.372	0.861	55.08	3.817	0.690	6.930
Gain:feed (7-14d)	92	81.77	2.431	0.822	82.26	2.534	0.851	3.080
Gain:feed (14-21d)	94	80.05	2.319	0.812	80.21	2.280	0.807	2.842
Gain:feed (21-28d)	88	71.71	1.101	0.893	70.92	3.598	0.265	5.073
Total gain:feed	89	75.69	1.408	0.888	75.50	2.409	0.754	3.190
<i>In vivo</i> viscosity	92	6.49	1.376	0.478	6.00	1.660	0.314	27.649
ME:GE	96	75.08	0.798	0.641	75.08	1.63	0.13	2.17
AME Content	95	14.16	0.175	0.604	14.13	0.35	0.19	2.45
ME:Gain	91	18.69	0.496	0.689	18.56	0.73	0.43	3.95
DM Retention	96	72.12	0.744	0.622	72.20	1.454	0.252	2.013
Ileal DM Digestibility	93	70.27	1.904	0.276	69.66	3.257	0.004	4.675
Ileal Starch Digestibility	96	91.48	2.369	0.487	92.55	2.312	0.522	2.498
Ileal CP Digestibility	89	77.62	1.447	0.730	75.94	3.965	0.015	5.222

N = number of spectra in the calibration equation, Mean_{cal} = mean of calibration dataset, SEC = standard error of calibration, R² = coefficient of determination of the calibration, SEP = standard error of prediction, R²_{val} = correlation coefficient of the validation, Mean_{val} = mean of independent validation set.

Table 8. Range and standard deviation of all wheats (including the Canadian wheats)

Variable	Units	Mean	Min	Max	Std Dev	No of Samples
Specific weight	kg/hl	70.72	59.00	78.00	4.03	138
Thousand grain weight	g	43.11	21.70	60.80	7.85	159
<i>In vitro</i> viscosity	cp	12.40	3.20	44.00	6.50	163
Nitrogen	g/kg DM	20.17	12.49	32.74	3.68	163
NDF	g/kg DM	140.74	101.30	195.00	13.79	163
Starch	g/kg DM	632.82	547.10	719.00	35.34	163
Total NSP	g/kg DM	106.96	81.70	138.80	11.24	141
Soluble NSP	g/kg DM	23.52	8.40	38.00	5.39	141
Lysine	g/kg DM	3.51	1.80	5.80	0.59	141
Threonine	g/kg DM	3.31	1.20	4.90	0.70	141
Gross Energy	MJ/kg DM	18.40	18.06	18.84	0.15	163
Amylose	g/kg DM	159.05	115.00	182.30	11.47	141
RSD (0.125h)	% starch	36.31	20.41	51.60	6.86	163
RSD (0.250h)	% starch	48.04	29.90	67.12	7.31	163
RSD (0.375h)	% starch	58.04	38.98	74.64	7.40	163
RSD (0.5h)	% starch	66.51	46.05	83.02	8.16	163
RSD (0.75h)	% starch	80.52	57.95	98.90	7.82	163
RSD (1h)	% starch	89.32	70.06	100.82	6.22	163
RSD (2h)	% starch	102.41	93.61	110.62	3.33	163
RSD Rate Constant	% degradation/h	2.51	1.33	4.35	0.60	163
Hardness	*	35.68	8.41	66.65	12.80	107
Protein profile (Band 1)	%	5.05	2.10	7.90	1.08	84
Protein profile (Band 2)	%	14.47	9.10	18.80	2.06	84
Protein profile (Band 3)	%	18.37	10.20	23.60	3.48	84
Protein profile (Band 4)	%	35.39	24.30	48.10	4.43	84
Protein profile (Band 5)	%	26.60	20.90	37.40	3.30	84
DMI (7-14d)	g/d	34.38	28.80	39.30	2.40	93
DMI (14-21d)	g/d	71.51	58.60	83.10	4.73	93
DMI (21-28d)	g/d	115.25	92.20	134.90	8.84	93
Total DMI	g/d	73.77	61.60	85.70	4.94	93
LWG (7-14d)	g/d	28.52	21.40	33.20	3.34	93
LWG (14-21d)	g/d	57.47	42.40	65.10	5.90	93
LWG (21-28d)	g/d	81.84	58.10	96.30	8.45	93
Total LWG	g/d	55.93	41.90	64.20	5.67	93
Gain:feed (7-14d)	*	82.75	73.10	90.60	5.06	93
Gain:feed (14-21d)	*	80.41	71.90	88.40	4.40	93
Gain:feed (21-28d)	*	71.11	61.50	78.20	3.20	93
Total gain:feed	*	75.79	67.20	81.70	3.59	93
<i>In vivo</i> viscosity	cp	5.89	3.31	12.98	1.97	93
ME:GE ratio	*	73.81	67.10	78.40	2.30	93
AME Content	MJ/kg DM	13.92	12.67	14.79	0.46	93
ME:Gain ratio	MJ/kg	18.31	16.72	20.86	0.90	93
DM Retention	%	72.13	69.70	75.30	1.31	61
Ileal DM Digestibility	%	69.98	62.70	75.60	2.66	61
Ileal Starch Digestibility	%	91.71	83.20	97.20	3.30	61
Ileal CP Digestibility	%	76.92	70.30	83.20	3.26	61

* = no units, R^2_{cv} = correlation coefficient of cross validation.

Table 9(a). *NIRS full calibration statistics for dried milled wheat, including Canadian samples*

Variable	N	Mean	SEC	R ²	SECV	R ² _{cv}	Terms	SECV as % of mean
Thousand grain weight	313	43.31	3.487	0.796	4.193	0.705	11	9.68
<i>In vitro</i> viscosity	313	11.59	2.796	0.693	3.044	0.635	9	26.28
Nitrogen	309	20.05	0.283	0.994	0.335	0.991	11	1.67
NDF	315	140.36	7.935	0.616	8.926	0.517	8	6.36
Starch	316	632.32	13.086	0.861	15.296	0.809	11	2.42
Gross Energy	316	18.40	0.052	0.873	0.055	0.858	6	0.30
RSD (0.125h)	313	36.25	2.427	0.871	2.947	0.810	11	8.13
RSD (0.250h)	318	47.92	2.898	0.837	3.276	0.791	10	6.84
RSD (0.375h)	313	58.05	2.884	0.845	3.282	0.799	10	5.65
RSD (0.5h)	321	66.49	3.258	0.838	3.734	0.787	10	5.62
RSD (0.75)	314	80.57	2.818	0.867	3.276	0.820	11	4.07
RSD (1h)	321	89.35	2.483	0.836	3.041	0.754	11	3.40
RSD (2h)	317	102.54	1.731	0.720	2.034	0.613	11	1.98
RSD Rate Constant	315	2.48	0.216	0.858	0.260	0.795	10	10.47

N = number of spectra in the calibration equation, SEC = standard error of calibration, RSQ = coefficient of determination of the calibration, SECV = standard error of cross validation, R²_{cv} = coefficient of cross validation, factors = number of actual terms used to estimate the parameter.

Table 9(b). NIR sub-calibration and true validation statistics for chemical and physical parameters of dried milled wheat, including Canadian samples

Variable	N	Mean _{cal}	SEC	R ²	Mean _{val}	SEP	R ² _{val}	SEP as % of Mean _{val}
Thousand grain weight	245	43.19	3.101	0.850	43.44	5.44	0.505	12.52
<i>In vitro</i> viscosity	248	11.62	2.979	0.641	12.60	6.69	0.262	53.05
Nitrogen	245	20.01	0.291	0.993	20.38	0.77	0.957	3.80
NDF	245	139.56	6.325	0.771	142.33	11.41	0.957	8.02
Starch	249	632.62	13.581	0.843	632.36	25.29	0.216	4.00
Gross Energy	256	18.39	0.052	0.865	18.40	0.04	0.571	0.24
RSD (0.125h)	249	35.72	2.152	0.894	38.00	4.59	0.914	12.07
RSD (0.250h)	248	47.33	2.462	0.876	50.15	5.23	0.658	10.42
RSD (0.375h)	249	57.51	2.908	0.841	60.12	4.83	0.592	8.04
RSD (0.5h)	255	66.09	2.886	0.877	68.12	4.37	0.632	6.41
RSD (0.75)	254	80.23	2.690	0.877	82.02	3.63	0.680	4.43
RSD (1h)	250	89.05	2.553	0.833	90.70	3.71	0.737	4.09
RSD (2h)	257	102.27	1.550	0.770	103.27	3.33	0.632	3.23
RSD Rate Constant	252	2.43	0.170	0.904	2.66	0.37	0.122	13.85

N = number of spectra in the calibration equation, Mean_{cal} = mean of calibration dataset, SEC = standard error of calibration, R² = coefficient of determination of the calibration, SEP = standard error of prediction, R²_{val} = correlation coefficient of the validation, Mean_{val} = mean of independent validation set.

Table 10(a). *NIRS full calibration statistics for undried milled wheat, including Canadian samples*

Variable	N	Mean	SEC	R ²	SECV	R ² _{cv}	Factors	SECV as % of Mean
Thousand grain weight	317	43.14	3.363	0.815	4.183	0.714	11	9.70
<i>In vitro</i> viscosity	305	11.28	2.579	0.701	2.830	0.639	9	25.09
Nitrogen	309	20.14	0.330	0.991	0.389	0.988	10	1.93
NDF	319	140.71	8.613	0.597	9.569	0.509	8	6.80
Starch	314	632.18	14.189	0.839	16.703	0.776	10	2.64
Gross Energy	320	18.40	0.046	0.904	0.056	0.860	9	0.30
RSD (0.125h)	317	36.10	3.013	0.797	3.197	0.771	7	8.86
RSD (0.250h)	309	47.86	3.143	0.797	3.181	0.791	7	6.65
RSD (0.375h)	318	57.96	3.109	0.815	3.679	0.740	10	6.35
RSD (0.5h)	319	66.51	3.330	0.831	3.802	0.779	10	5.72
RSD (0.75h)	316	80.63	3.212	0.826	3.640	0.776	9	4.51
RSD (1h)	324	89.43	2.713	0.800	3.250	0.713	10	3.63
RSD (2h)	309	102.58	1.930	0.627	2.067	0.571	7	2.01
RSD Rate Constant	306	2.47	0.214	0.853	0.241	0.813	9	9.75

N = number of spectra in the calibration equation, SEC = standard error of calibration, RSQ = coefficient of determination of the calibration, SECV = standard error of cross validation, R²_{cv} = coefficient of cross validation, factors = number of actual terms used to estimate the parameter.

Table 10(b). NIR sub-calibration and true validation statistics for chemical and physical parameters of undried milled wheat, including Canadian samples

Variable	N	Mean _{cal}	SEC	R ²	Mean _{val}	SEP	R ² _{val}	SEP as % of Mean _{val}
Thousand grain weight	248	43.23	3.722	0.781	43.44	5.77	0.481	13.29
<i>In vitro</i> viscosity	241	11.25	2.499	0.707	12.60	6.24	0.497	49.48
Nitrogen	251	20.10	0.375	0.989	20.38	0.78	0.956	3.81
NDF	250	139.70	7.089	0.704	142.33	10.04	0.956	7.05
Starch	252	632.94	13.412	0.850	632.36	26.60	0.308	4.21
Gross Energy	256	18.39	0.051	0.879	18.40	0.05	0.536	0.27
RSD (0.125h)	249	35.84	2.322	0.883	38.00	4.37	0.895	11.49
RSD (0.250h)	248	47.40	2.689	0.846	50.15	4.72	0.685	9.42
RSD (0.375h)	249	57.45	2.874	0.840	60.12	4.91	0.648	8.17
RSD (0.5h)	251	66.12	2.936	0.869	68.12	4.61	0.600	6.77
RSD (0.75h)	250	80.13	2.768	0.873	82.02	4.25	0.642	5.19
RSD (1h)	254	89.19	2.678	0.808	90.70	3.36	0.655	3.70
RSD (2h)	246	102.44	1.801	0.681	103.27	2.89	0.665	2.80
RSD Rate Constant	246	2.42	0.172	0.901	2.66	0.37	0.279	13.79

N = number of spectra in the calibration equation, Mean_{cal} = mean of calibration dataset, SEC = standard error of calibration, R² = coefficient of determination of the calibration, SEP = standard error of prediction, R²_{val} = correlation coefficient of the validation, Mean_{val} = mean of independent validation set

Figure 1. Comparison of actual and NIRS predicted nitrogen values for dried and undried milled wheat samples, excluding Canadian wheat

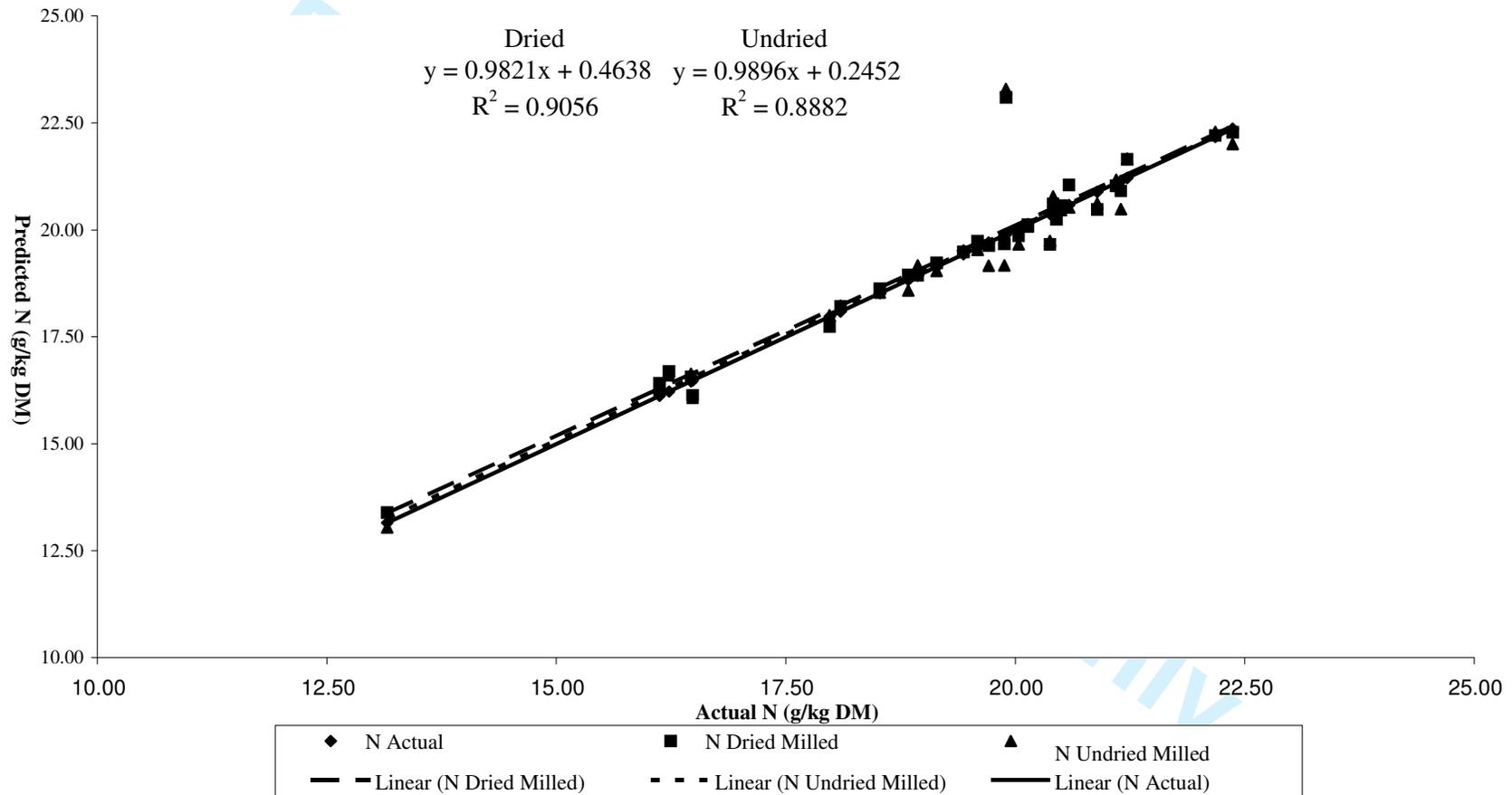


Figure 2. Comparison of actual and NIRS predicted rate of starch digestion (RSD) values for dried and undried milled wheat samples, excluding Canadian wheat

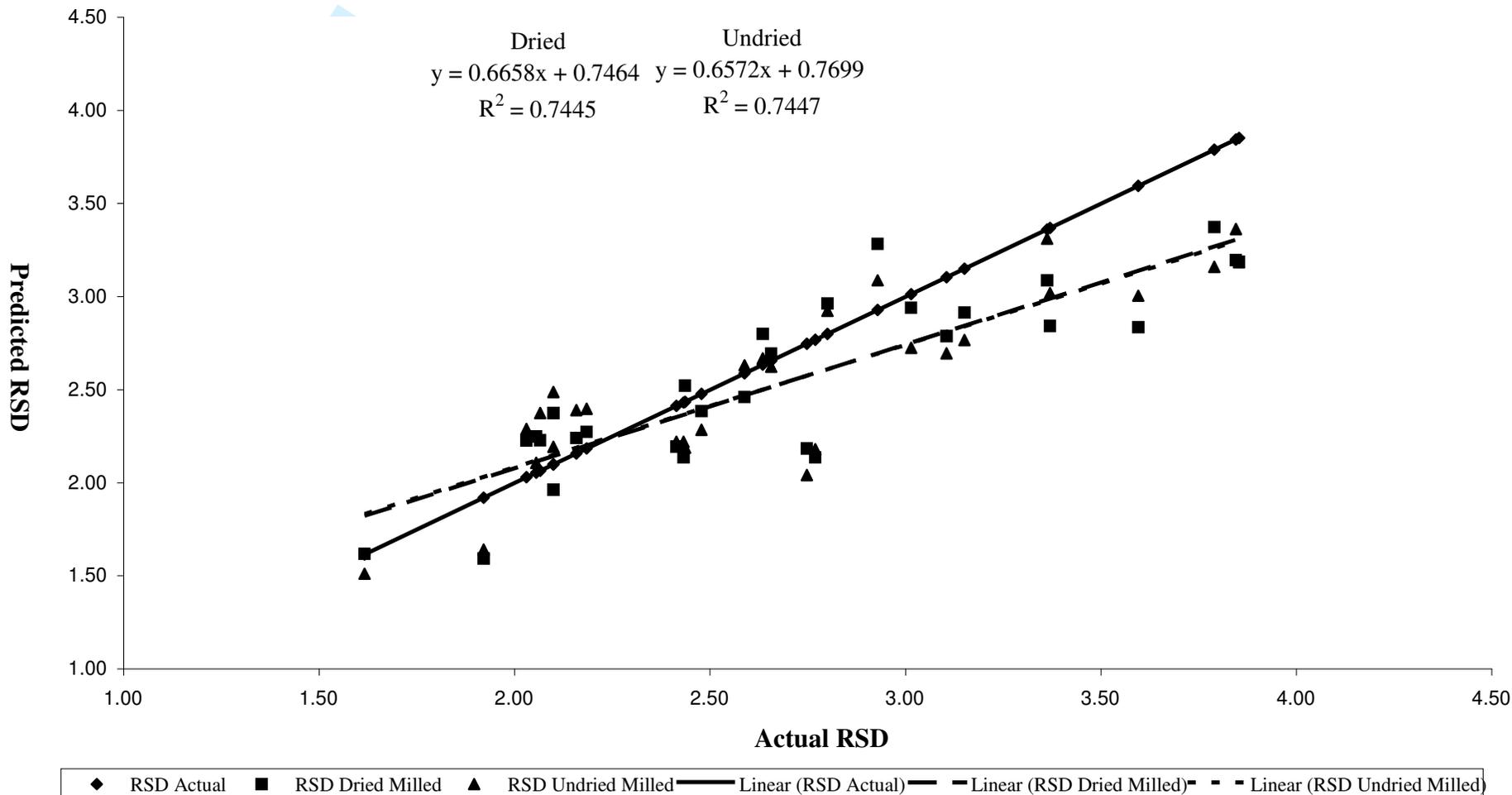


Figure 3. Comparison of actual and NIRS predicted total live weight gain (LWG) for dried and undried whole wheat samples

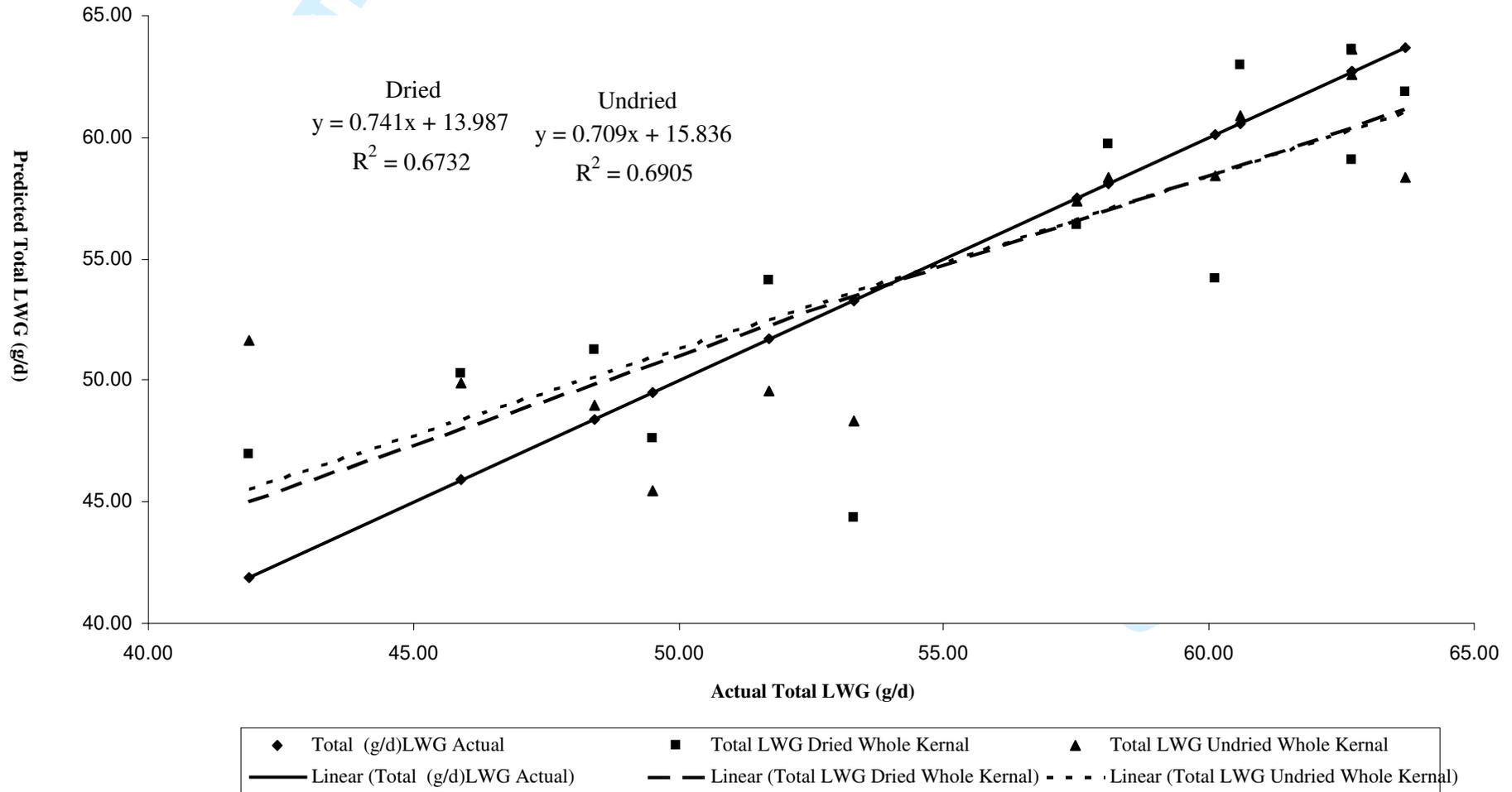


Figure 4. Comparison of actual and NIRS predicted total gain:feed for dried and undried whole wheat samples

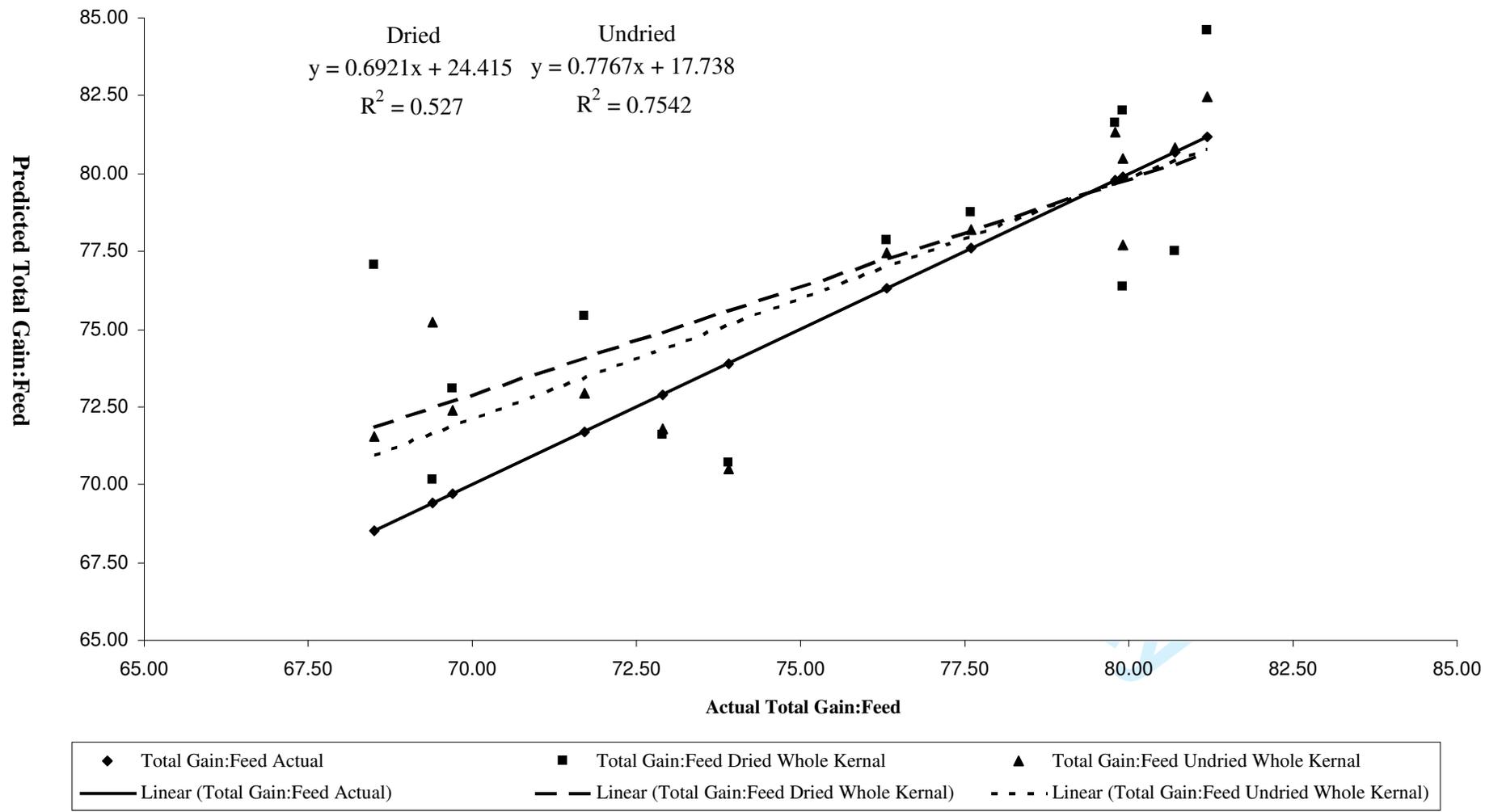


Figure 5. Comparison of actual and NIRS predicted gross energy (GE) values for dried and undried wheat samples, including Canadian

