Barley Straw: Component Evaluation Using the Cornell Net Carbohydrate and Protein System and Prediction of Nutritional Value by Near-Infrared Spectroscopy (Postprint)

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Date: 2018-12-24T00:00:00+00:00

Abstract

This study aimed to establish a nutritional component database for barley straw based on the Cornell Net Carbohydrate and Protein System (CNCPS) and develop a nutritional value prediction model using Near-Infrared Spectroscopy (NIRS). A total of 96 barley straw samples were collected from 13 counties and cities in Gansu Province to determine their dry matter (DM), crude ash (Ash), crude protein (CP), ether extract (EE), neutral detergent fiber (NDF), acid detergent fiber (ADF), acid detergent lignin (ADL), neutral detergent insoluble protein (NDIP), acid detergent insoluble protein (ADIP), soluble crude protein (SP), calcium (Ca), and phosphorus (P) contents. CNCPS 6.5 was utilized to calculate the carbohydrate (CHO) and protein nutritional components of each sample. Seventy-six and twenty barley straw samples were used as calibration and validation sets, respectively, to evaluate the NIRS prediction models. The results showed: 1) The DM, Ash, CP, EE, NDF, ADF, ADL, NDIP, ADIP, SP, Ca, and P contents of barley straw were 95.21%, 7.38%, 3.51%, 5.68%, 70.95%, 45.16%, 5.17%, 1.02%, 0.57%, 1.65%, 0.71%, and 0.09%, respectively. 2) The CNCPS CHO components of barley straw, namely CHO, non-fibrous carbohydrate (NFC), soluble fiber (CB2), digestible fiber (CB3), and indigestible fiber (CC), were 83.42%, 12.47%, 12.47%, 58.55%, and 12.40%, respectively. The CNCPS protein components of barley straw, namely soluble true protein (PA2), insoluble true protein (PB1), fiber-bound protein (PB2), and non-degradable protein (PC), were 1.65%, 1.23%, 0.45%, and 0.57%, respectively. 3) The cross-validation coefficient of determination (1-VR) for organic matter (OM), CP, NDF, ADF, CHO, NFC, and CB2 was >0.8, and the validation coefficient of determination (RSQv) was $ $0.84, indicating that these models could be used for routine analysis. The model parameters for OM, CP, NDF, ADF, CHO, NFC, and CB2 were standard normal variate and detrend second derivative treatment (SNV and detrend 2,4,4,1), SNV and detrend 2,4,4,1; standard normal variate and detrend first derivative treatment (SNV and detrend 1,4,4,1); no scatter first derivative treatment (None 1,4,4,1); SNV and detrend 2,4,4,1; no scatter second derivative treatment (None 2,4,4,1); None 2,4,4,1, respectively. However, the models established for the remaining components did not reach a practical level and require further improvement. In conclusion, this study provides basic chemical analysis data for the application of barley straw in ruminant diets and establishes rapid prediction models for major nutritional components through the NIRS method.

Full Text

Barley Straw: Evaluation of Components Using the Cornell Net Carbohydrate and Protein System and Prediction of Nutritional Value by Near-Infrared Spectroscopy

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Abstract

This study aimed to establish a nutritional component database for barley straw based on the Cornell Net Carbohydrate and Protein System (CNCPS) and develop predictive models for its nutritional value using near-infrared spectroscopy (NIRS). A total of 96 barley straw samples were collected from 13 counties and cities in Gansu Province. The contents of dry matter (DM), crude ash (Ash), crude protein (CP), ether extract (EE), neutral detergent fiber (NDF), acid detergent fiber (ADF), acid detergent lignin (ADL), neutral detergent insoluble protein (NDIP), acid detergent insoluble protein (ADIP), soluble protein (SP), calcium (Ca), and phosphorus (P) were determined. Carbohydrate (CHO) and protein nutritional components for each sample were calculated using CNCPS 6.5. The NIRS prediction models were evaluated using 76 samples for calibration and 20 samples for validation. The results showed that: (1) The DM, Ash, CP, EE, NDF, ADF, ADL, NDIP, ADIP, SP, Ca, and P contents of barley straw were 95.21%, 7.38%, 3.51%, 5.68%, 70.95%, 45.16%, 5.17%, 1.02%, 0.57%, 1.65%, 0.71%, and 0.09%, respectively. (2) The CNCPS CHO components of barley straw—CHO, non-fiber carbohydrates (NFC), soluble fiber (CB2), digestible fiber (CB3), and indigestible fiber (CC)—were 83.42%, 12.47%, 12.47%, 58.55%, and 12.40%, respectively. The CNCPS protein components—soluble true protein (PA2), insoluble true protein (PB1), fiber-bound protein (PB2), and non-degradable protein (PC)—were 1.65%, 1.23%, 0.45%, and 0.57%, respectively. (3) For organic matter (OM), CP, NDF, ADF, CHO, NFC, and CB2, the cross-validation coefficient (1-VR) exceeded 0.8 and the validation coefficient of determination (RSQv) was \$ \$0.84, indicating these models are suitable for routine analysis. The optimal model parameters were: SNV and detrend 2,4,4,1 for OM and CP; SNV and detrend 1,4,4,1 for NDF; None 1,4,4,1 for ADF; SNV and detrend 2,4,4,1 for CHO; None 2,4,4,1 for NFC and CB2. Models for other components did not reach practical applicability and require further improvement. In conclusion, this study provides fundamental chemical analysis data for the application of barley straw in ruminant diets and establishes rapid prediction models for major nutritional components using NIRS.

Keywords: barley straw; Cornell Net Carbohydrate and Protein System; near-infrared spectroscopy; nutritional value

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Introduction

Efficient utilization of straw resources represents a key research focus in ruminant nutrition. China possesses abundant barley straw resources, yet fundamental research on barley straw nutritional value databases remains scarce. Accurate assessment of nutritional value is essential for improving comprehensive utilization of barley straw resources, requiring both efficient and precise evaluation methods. The Cornell Net Carbohydrate and Protein System (CNCPS) has been widely applied in China for determining and evaluating the nutritional value of ruminant feeds, offering more comprehensive reflection of feed nutritional value compared to proximate analysis systems, particularly in analyzing fiber components and assessing potential feeding value of roughages. Near-infrared reflectance spectroscopy (NIRS) has been extensively employed in detecting nutritional composition of ruminant forages, enabling rapid and accurate prediction of multiple nutritional parameters compared to traditional chemical analysis methods. This study analyzed barley straw nutritional components based on CNCPS to provide fundamental data for practical production. Additionally, NIRS was utilized to establish calibration models for nutritional components in barley straw samples, with external validation performed to determine model feasibility for rapid nutritional value assessment in production settings.

Materials and Methods

1.1 Sample Collection and Preparation A total of 96 barley straw samples were collected from Yongdeng County, Tianzhu Tibetan Autonomous County, Jingtai County, Gulang County, Wuwei City, Minqin County, Yongchang County, Jinchang City, Shandan County, Zhangye City, Minle County, Sunan Yugur Autonomous County, and Yumen City in Gansu Province. Representative whole-plant mature barley straw samples (1.5–2.0 kg) free from mold and weeds were selected according to Feed Hygiene Standards. Sample collection information cards were prepared concurrently, recording straw name, variety, sampling date, grain harvest date, location, and collector, and placed with samples in collection bags.

Collected whole-plant barley straw samples were chopped to 3–5 cm lengths and ground using a cutting mill (SM-2000). The ground material was passed through a 40-mesh sieve, thoroughly mixed, sealed in self-locking bags, and stored for analysis.

1.2.1 Proximate Nutrient Analysis Dry matter (DM), crude protein (CP), ether extract (EE), crude ash (Ash), and starch contents were determined according to reference [6]. Neutral detergent fiber (NDF), acid detergent fiber (ADF), acid detergent lignin (ADL), neutral detergent insoluble protein (NDIP), and acid detergent insoluble protein (ADIP) were measured using the method of Van Soest et al. [7]. Soluble crude protein (SP) content was determined according to Krishnamoorthy et al. [8]. Calcium (Ca) was measured by air-acetylene flame atomic absorption spectrometry [9], and phosphorus (P) by ammonium vanadomolybdate spectrophotometry [10]. All samples were analyzed in triplicate.

1.2.2 CNCPS Classification and Calculation Methods CNCPS is a dynamic rumen fermentation prediction model for dairy cattle developed through extensive scientific research at Cornell University. This evaluation system correlates feed chemical composition with rumen digestion characteristics based on degradation properties, enabling prediction of feed nutritional value and dairy cattle performance. CNCPS provides deeper assessment of feed carbohydrate (CHO) and protein nutritional value [7].

The 2015 version, CNCPS 6.5, divides CHO into three fractions: CA, CB, and indigestible fiber (CC) [11]. CA includes volatile fatty acids (CA1), lactic acid (CA2), other organic acids (CA3), and water-soluble carbohydrates (CA4). CB includes starch (CB1), soluble fiber (CB2), and digestible fiber (CB3). CA, CB1, and CB2 constitute non-fiber carbohydrates (NFC). CC is 2.4 times ADL, while CB3 and CC represent fibrous carbohydrates (FC). Calculations are as follows:

CHO (%DM) = 100 - CP (%DM) - EE (%DM) - Ash (%DM)
NFC (%DM) = CHO (%DM) - NDF (%DM)

CB2 (%DM) = NFC (%DM) - CA1 (%DM) - CA2 (%DM) - CA3 (%DM) - CA4 (%DM) - CB1 (%DM)
CB3 = NDF (%DM) - CC (%DM)
CC (%DM) = {NDF (%DM) × [ADL (%NDF) × NDF (%DM)] × 2.4} / 100

In the CNCPS 6.5 protein system, feed protein is divided into three fractions: PA, PB, and non-degradable protein (PC). PA includes ammonia (PA1) and soluble true protein (PA2), while PB includes insoluble true protein (PB1) and fiber-bound protein (PB2). Calculations are:

PA1 (%DM) = ammonia (%SP) × [SP (%CP) / 100] × [CP (%DM)] / 100
PA2 (%DM) = [SP (%CP) × CP (%DM)] / 100 - PA1 (%DM)
PB1 (%DM) = CP (%DM) - PA1 (%DM) - PA2 (%DM) - PB2 (%DM) - PC (%DM)
PB2 = [NDICP (%CP) - ADICP (%CP)] × CP (%DM) / 100
PC = ADICP (%CP) × CP (%DM) / 100

1.3.1 NIRS Equipment and Software A DS-2500 near-infrared spectrometer (FOSS, USA) was used, with data acquisition frequency of 2 Hz, spectral resolution of 2 nm, and wavelength accuracy less than 0.05 nm. Samples were packed to ensure uniform flatness and compaction. Data were collected using ISIscan Nova 5.5 software, with model calibration and validation performed using WinISI III software [12–14].

1.3.2 NIRS Analysis Methods After principal component regression (PCR) of barley straw samples, Mahalanobis distance was calculated for calibration and validation. This study primarily utilized scatter correction combining SNV and detrend with PCR mathematical processing to eliminate sample or external interference during NIRS acquisition, reduce baseline drift or offset, and improve spectral accuracy and resolution. This approach enabled selection of scientifically reasonable principal components for effective prediction of sample components in complex analytical systems without prior knowledge of interfering components.

1.3.3 NIRS Spectral Evaluation Parameters Calibration and validation sets were selected at a 4:1 ratio [14], comprising 76 and 20 barley straw samples, respectively. Samples with nutrient content between maximum and minimum values were selected for calibration [4]. Calibration evaluation parameters included standard error of calibration (SEC), standard error of cross-validation (SECV), and 1 minus the variance ratio (1-VR), determined according to Li Yupeng [13] and Zhou Junqin [14]. Validation parameters included standard error of prediction (SEP), coefficient of determination for validation (RSQv), and bias, determined according to Li Yupeng [13], Zhou Junqin [14], Malley [15], and Li Junxia [16]. Optimal model establishment followed methods from Chu Xiaoli [17] and Li Juntao [18].

1.3.4 NIRS Evaluation Parameter Calculation Methods **SEC:** Standard deviation between chemical measured values and NIRS predicted values obtained by applying the calibration model to the calibration sample set [17].

SECV: Standard deviation between NIRS predicted values and chemical measured values during cross-validation in model development, providing approximate assessment of prediction accuracy [17].

1-VR: Correlation coefficient obtained during cross-validation, representing the percentage of sample set concentration variation explained by the model. A 1-VR value of 1 indicates 100% explanation of calibration set concentration variation during cross-validation [17].

SEP: Alarm limit is 1.3 times the equation error SEC [17].

RSQv: Percentage of calibration sample set variation explained by the model. An RSQv of 1 indicates 100% explanation of calibration set concentration variation [17]. RSQv returns r^2 (square of correlation coefficient r), where r is calculated as:

Bias: Alarm limit is 0.6 times the calibration error SEC [17].

1.4 Statistical Analysis Data were subjected to descriptive statistics using SPSS 16.0. Paired t-tests and regression analysis were performed on analytical and predicted values from validation samples, with significance set at $P < 0.05$.

Results

2.1 Conventional Nutrient Content of Barley Straw As shown in Table 1 , barley straw DM content ranged from 93.63% to 97.27% (mean 95.21%); Ash from 4.21% to 11.57% (mean 7.38%); CP from 2.01% to 7.83% (mean 3.51%); EE from 2.88% to 8.34% (mean 5.68%); NDF from 58.74% to 79.91% (mean 70.95%); ADF from 29.85% to 54.13% (mean 45.16%); ADL from 1.44% to 14.10% (mean 5.17%); NDIP from 0.61% to 1.75% (mean 1.02%); ADIP from 0.27% to 0.97% (mean 0.57%); SP from 0.12% to 5.99% (mean 1.65%); Ca from 0.57% to 0.99% (mean 0.71%); and P from 0.04% to 0.17% (mean 0.09%).

Table 1 Nutritional components of barley straw (DM basis)

Items	Maximum	Minimum	%
Dry matter DM			
Crude ash Ash			
Crude protein CP			
Ether extract EE			
Neutral detergent fiber NDF			
Acid detergent fiber ADF			

Items	Maximum	Minimum	%
Acid detergent lignin ADL			
Neutral detergent insoluble protein NDIP			
Acid detergent insoluble protein ADIP			
Soluble crude protein SP			

2.2 CNCPS Component Content of Barley Straw As shown in Table 2 , barley straw CHO content ranged from 77.07% to 89.79% (mean 83.42%), and NFC content from 5.61% to 20.26% (mean 12.47%).

Within the CHO system, CB2 ranged from 5.61% to 20.26% (mean 12.47%); CB3 from 33.57% to 70.36% (mean 58.55%); and CC from 3.47% to 33.84% (mean 12.40%). In the protein system, PA2 ranged from 0.12% to 5.99% (mean 1.65%); PB1 from 0.19% to 2.97% (mean 1.23%); PB2 from 0.00% to 1.20% (mean 0.45%); and PC from 0.27% to 0.97% (mean 0.57%). Components CA1, CA2, CA3, CA4, CB1, and PA1 were not detected (0.00%), with small variation coefficients for all components.

Table 2 The CNCPS nutritional components of barley straw (DM basis)

Items	Maximum	Minimum
Carbohydrate CHO		
Non-fiber carbohydrates NFC		
Volatile fatty acids CA1		
Lactic acid CA2		
Other organic acids CA3		
Water-soluble carbohydrates CA4		
Starch CB1		
Soluble fiber CB2		
Digestible fiber CB3		
Indigestible fiber CC		
Ammonia PA1		
Soluble true protein PA2		
Insoluble true protein PB1		
Fiber-bound protein PB2		
Non-degradable protein PC		

2.3 NIRS Spectra of Barley Straw Second-derivative processed spectra of 96 barley straw samples were scanned using a DS-2500 spectrometer, as shown in Figure 1 [Figure 1: see original paper].

Figure 1 Second derivative processed NIRS spectrum (n=96)

2.4 Establishment of NIRS Models for Barley Straw Nutrients As shown in Table 3 , SECV values were 0.0037 for OM (1-VR = 0.9526), 0.0021 for CP (1-VR = 0.9448), 0.0102 for NDF (1-VR = 0.9468), 0.0128 for ADF (1-VR = 0.9033), 0.0073 for CHO (1-VR = 0.9209), 0.0107 for NFC (1-VR = 0.8571), and 0.0107 for CB2 (1-VR = 0.8571). For other nutrients, 1-VR values were <0.8, rendering these models unsuitable for external validation.

Table 3 Parameters of optimal NIRS model of barley straw nutritional components

Items	NIRS model parameters	SEC	SECV	1-VR
Dry matter DM	SNV and detrend 2,4,4,1			
Organic matter OM	SNV and detrend 2,4,4,1			
Crude protein CP	SNV and detrend 2,4,4,1			
Ether extract EE	None 2,4,4,1			
Neutral detergent fiber NDF	SNV and detrend 1,4,4,1			
Acid detergent fiber ADF	None 1,4,4,1			
Acid detergent lignin ADL	SNV and detrend 1,4,4,1			
Neutral detergent insoluble protein NDIP	SNV and detrend 1,4,4,1			
Acid detergent insoluble protein ADIP	SNV and detrend 1,4,4,1			

Items	NIRS model parameters	SEC	SECV	1-VR
Soluble crude protein SP	SNV and detrend 2,4,4,1			
Carbohydrate CHO	SNV and detrend 2,4,4,1			
Non-fiber carbohydrates NFC	None 2,4,4,1			
Soluble fiber CB2	None 2,4,4,1			
Digestible fiber CB3	SNV and detrend 2,4,4,1			
Indigestible fiber CC	SNV and detrend 1,4,4,1			
Soluble true protein PA2	None 2,4,4,1			
Insoluble true protein PB1	SNV and detrend 2,4,4,1			
Fiber-bound protein PB2	None 1,4,4,1			
Non-degradable protein PC				

2.5 External Validation of Barley Straw Nutrient NIRS Models Based on SEP, RSQv, and bias, optimal models were externally validated using the calibration set to evaluate NIRS prediction accuracy and practical applicability. As shown in Table 4 and Figures 2 [Figure 2: see original paper] through 8 [Figure 8: see original paper], RSQv values were 0.981 for DM, 0.925 for OM, 0.920 for CP, 0.872 for EE, 0.868 for NDF, 0.877 for ADF, 0.890 for NDIP, 0.960 for ADIP, 0.865 for SP, 0.975 for CHO, 0.878 for NFC, 0.878 for CB2, 0.843 for PA2, 0.840 for PB2, and 0.902 for PC. With RSQv $ $0.84, these models are considered suitable for routine analysis. Models for remaining components (RSQv <0.84) are not suitable for practical application.

Table 4 Parameters of optimal NIRS model of barley straw nutritional components for external validation

Items	SEP	RSQv
Dry matter DM		
Organic matter OM		
Crude protein CP		
Ether extract EE		
Neutral detergent fiber NDF		
Acid detergent fiber ADF		
Acid detergent lignin ADL		
Neutral detergent insoluble protein NDIP		
Acid detergent insoluble protein ADIP		
Soluble crude protein SP		
Carbohydrate CHO		
Non-fiber carbohydrates NFC		
Soluble fiber CB2		
Digestible fiber CB3		
Indigestible fiber CC		
Soluble true protein PA2		
Insoluble true protein PB1		
Fiber-bound protein PB2		
Non-degradable protein PC		

LAB: measured value; NIR: NIRS predictive value. The same as below.

Figure 2 Regression between measured value of the validation OM and NIRS predictive value (paired t test, n=17, P=0.188)

Figure 3 Regression between measured value of the validation CP and NIRS predictive value (paired t test, n=16, P=0.164)

Figure 4 Regression between measured value of the validation NDF and NIRS predictive value (paired t test, n=14, P=0.205)

Figure 5 Regression between measured value of the validation ADF and NIRS predictive value (paired t test, n=17, P=0.548)

Figure 6 Regression between measured value of the validation CHO and NIRS predictive value (paired t test, n=10, P=0.343)

Figure 7 Regression between measured value of the validation NFC and NIRS predictive value (paired t test, n=20, P=0.095)

Figure 8 Regression between measured value of the validation CB2 and NIRS predictive value (paired t test, n=20, P=0.095)

Discussion

3.1 Conventional Nutrients in Barley Straw As a primary roughage source for ruminants, barley straw in this study contained DM, Ash, CP, NDF, ADF, and ADL at 95.21%, 7.38%, 3.51%, 70.95%, 45.16%, and 5.17%, respectively. Lü Zhenwu et al. [19] reported Tibetan naked barley straw contained 89.57% DM, 8.01% Ash, 2.07% CP, 69.85% NDF, 49.42% ADF, and 8.56% ADL. Compared with their results, our study showed lower Ash, ADF, and ADL but higher DM, CP, and NDF contents.

3.2 Characteristics of CNCPS Nutrients in Barley Straw Barley straw CHO content was 83.42%, with CB3 being the highest fraction at 58.55%. CB3 represents utilizable plant cell walls that undergo relatively slow degradation in the rumen and is abundant in roughages such as corn stalks and grasses [20]. Components CA1, CA2, CA3, CA4, and CB1 were not detected in barley straw samples.

Zhang Peng et al. [21] reported that PC in straw primarily binds with ADL and remains undegraded in both rumen and hindgut; lower PC content indicates higher barley straw utilization. In this study, protein fractions PA1, PA2, PB1, PB2, and PC were 0.00%, 1.65%, 1.23%, 0.45%, and 0.57%, respectively. The low PC content suggests high protein utilization in ruminants. The relatively high PA2 content aligns with reports from Zhao Guangyong [22] and Li Jianyun [23] that non-protein nitrogen constitutes the main soluble protein fraction in roughages.

3.3 NIRS Prediction of Barley Straw Nutrients Extensive research has been conducted on NIRS analysis of roughage nutrients. Generally, NIRS models require RSQv $ $0.84 [12] and 1-VR >0.8 [15] for practical use. This study successfully established models for four proximate nutrients: OM, CP, NDF, and ADF. However, other components showed RSQv $ $0.84 and 1-VR <0.8, indicating need for further optimization. Prediction models for CP, CF, and Ash in roughages are relatively mature, with multiple successful reports. Modroño et al. [24] developed robust CP and CF prediction models using portable NIRS (1-VR = 0.88–0.90 and 0.85–0.91, respectively). Bruno et al. [25] reported validation coefficients >0.9 for CP, NDF, ADF, and Ash in ryegrass. Wang Fangbin [4] established NIRS models for DM and CP in 125 rapeseed straw samples from Northwest China, though most other nutrients showed poor predictions. Belanche et al. [26] analyzed DM and NDF in 660 feed samples of 80 types post in situ degradation, achieving accurate NDF determination via partial least squares but poor DM prediction accuracy, consistent with our results for barley straw DM and NDF.

Limited reports exist on NIRS prediction of CNCPS nutrients. This study systematically compared NIRS models for barley straw CNCPS components, showing that CHO, NFC, and CB2 in the CHO system achieved RSQv $ $0.84 and 1-VR >0.80, making them suitable for production. However, CB3 and CC showed RSQv of 0.064 and 0.228, with 1-VR of 0.4564 and 0.5319, respectively. For PA2, PB2, and PC, RSQv values were 0.843, 0.840, and 0.902, respectively —superior to values of 0.054, 0.734, and 0.747 reported for forages by Valdés et al. [27]. Our results outperform those of Chen Long et al. [28], possibly due to broader geographic sampling and consistent collection timing in this study.

This study provides preliminary nutritional evaluation of barley straw via proximate analysis, followed by detailed CHO and protein fraction analysis using CNCPS to assess potential feeding value [11]. In practice, barley straw nutrient contents can be imported into CNCPS formulation software to predict ruminant performance [29].

Conclusion

1. Barley straw contained 95.21% DM, 7.38% Ash, 3.51% CP, 5.68% EE, 70.95% NDF, 45.16% ADF, 5.17% ADL, 1.02% NDIP, 0.57% ADIP, 1.65% SP, 0.71% Ca, and 0.09% P.
2. CNCPS nutrients in barley straw were: CHO 83.42%, NFC 12.47%, CB2 12.47%, CB3 58.55%, CC 12.40%, PA2 1.65%, PB1 1.23%, PB2 0.45%, and PC 0.57%.
3. NIRS prediction models were established with parameters: OM (SNV and detrend 2,4,4,1), CP (SNV and detrend 2,4,4,1), NDF (SNV and detrend 1,4,4,1), ADF (None 1,4,4,1), CHO (SNV and detrend 2,4,4,1), NFC (None 2,4,4,1), and CB2 (None 2,4,4,1). With 1-VR >0.8 and RSQv $ $0.84, these models enable rapid evaluation of these components in production settings.
4. This study provides fundamental chemical analysis data for barley straw application in ruminant diets and establishes rapid prediction models for major nutrients using NIRS.

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