Animal Feed Science and Technology 165 (2011) 111–119

Contents lists available at ScienceDirect

Animal Feed Science and Technology

journal homepage: www.elsevier.com/locate/anifeedsci

Nondestructive assessment of amino acid composition in rapeseed meal based on intact seeds by near-infrared reflectance spectroscopy

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ARTICLE INFO

Article history:
Received 20 January 2010
Received in revised form 25 January 2011
Accepted 4 February 2011

Keywords:
Near infrared reflectance spectroscopy (NIRS)
Amino acids content
Rapeseed meal
Intact rapeseed

ABSTRACT

The ability of near-infrared spectroscopy (NIRS) was tested for estimating individual and total amino acid contents in rapeseed meal. Twelve different amino acids (aspartic acid, threonine, serine, glutamic acid, glycine, isoleucine, leucine, tyrosine, phenylalanine, lysine, histidine and arginine) in rapeseed meal could be predicted. The R^2 ranged from 0.89 to 0.98, 1 – VR (1 minus the ratio of unexplained variance to total variance) ranged from 0.86 to 0.97 and the ratio of sample standard deviation (SD) to the standard error of cross-validation (SECV) ranged from 2.69 to 5.90. The equations for alanine showed better agreement between reference value and spectra (R^2 = 0.84, 1 – VR = 0.82 and SD/SECV = 2.15). The calibration model for proline (R^2 = 0.81 and 1 – VR = 0.78), methionine (R^2 = 0.80 and 1 – VR = 0.78), cysteine (R^2 = 0.76 and 1 – VR = 0.74), and valine (R^2 = 0.62 and 1 – VR = 0.58) however explained less variation. The NIRS prediction equation for total amino acid also showed high coefficient of determination (R^2 = 0.93) and SD/SECV (3.87), and low SECV (17.01 g/kg). Equations of 9 amino acids (aspartic acid, glutamic acid, glycine, alanine, valine, leucine, lysine, histidine and arginine) were developed for relative contents of total amino acid and deemed useful for prediction with R^2 values from 0.80 to 0.95, 1 – VR from 0.70 to 0.95 and SD/SECV from 1.83 to 3.95 and reasonably low SECV values. These results demonstrated that NIRS is a reliable tool for nondestructive assessment of variation in amino acid contents, increasing the efficiency of breeding and accelerating the selection process in rapeseed.

1. Introduction

Brassica oilseed crops are mainly grown for the production of vegetable oils which are used for human consumption or industrial applications and their byproduct are high protein feed meal which includes about 400 g/kg of crude protein. Rapeseed protein which has a rational amino acid composition is another important source of nutrition (Goding et al., 1972; Huisman and Tolman, 1990). The contents of two amino acids (methionine and cysteine) are higher than those in soybean and peanut. Soluble protein, lysine and other essential amino acid contents are also higher than those in sunflower and

Abbreviations: 1 – VR, 1 minus the ratio of unexplained variance to total variance; CV, the coefficient of variation; MPLS, modified partial least squares; NIRS, near infrared reflectance spectroscopy; R^2, coefficient of determination in calibration; RSD_r, relative standard deviation for repeatability; SD, standard deviation; SD/SECV, ratio of the standard deviation (SD) of the amino acid contents in the calibration samples to the standard error of cross-validation (SECV); SEC, the standard error of calibration; SECV, standard error of cross-validation; SNV + D, standard normal variate + detrending; S_r, repeatability of standard deviation; TAA, total of amino acids.

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doi:10.1016/j.anifeedsci.2011.02.004

sesame. The nutritional value of rapeseed meal is not less than that of soybean (Josefesson and Muhlenberg, 1968; Simbaya et al., 1995). Wu et al. (2005) found that protein content of rapeseed was simultaneously controlled by genetic effects of embryo, cytoplasm, and maternal plant, of which the maternal genetic effect was most important. The total narrow-sense heritability is high. Röbbelen (1981) pointed out that the development of high-protein cultivars in rapeseed is an important objective for breeding because the rapeseed meal can be transformed into good feed for livestock. High protein content and rational amino acids composition in rapeseed are major concern to the breeder.

Improvement for seed quality traits depends on the availability of fast and accurate methods for their measurement in breeding practice (Wu and Shi, 2004). Near infrared reflectance spectroscopy (NIRS) technique started in 1960s (Ben-Gera and Norris, 1968), has developed rapidly since late 1980s, and become a powerful green analytical tool for the routine analysis of quality traits in rapeseed. Using intact seeds sample, NIRS calibration equations have been confirmed to be useful to routinely determine simultaneously several quality traits, such as oil, protein and glucosinolate contents as well as fatty acid composition (Velasco et al., 1997; Velasco and Becker, 1998a,b; Velasco et al., 1999; Wu et al., 2002a). Velasco and Möllers (2002) reported that the NIRS technique was reliable enough for the estimation of protein content in a single rapeseed. Hom et al. (2007) compared the accuracy of NIRS analysis of protein and oil content in intact seeds sample size of 3–4 g with the same content in a single seed (5 mg), and concluded that standard NIRS calibration equations could be used for screening a single rapeseed. The method to determine the fatty acid composition of the seed oil at a half-seed level (Downey and Harvey, 1963) has been substituted by the above method for the improvement of seed oil quality.

Near-infrared spectroscopy has been used on intact grains of wheat (Abe et al., 1995; Roussel et al., 2005), milled rice flour (Wu et al., 2002b) and a single corn kernel (Baye et al., 2006) to predict nutrient quality traits such as protein and amino acid content. In the feed industry, quick and accurate analysis methods on contents of essential amino acids in the most important protein-rich feed draws a lot of attention from feed researchers. NIRS calibrations were developed for the accurate and fast determination of the total contents of important essential amino acids and protein with the finely ground material in the most cereals, bran and meals for animal feed production (Fontaine et al., 2001, 2002). Their equations facilitate the routine work, improve the accuracy of feed formulation and quality, and decrease production cost (Pujol et al., 2007). NIRS technique is widely applied in agricultural product analyses and breeding programs (Wu et al., 2002a,b).

Protein content is determined in the laboratory by a classical procedure of the Kjeldahl method, and amino acid content by the HCl hydrolysis-HPLC method. These conventional chemical analytical methods are time-consuming and expensive. They are also considered destructive because they require grinding and other pretreatments of samples which make them unsuitable for the analysis of a large number of samples in the early generations of breeding. A rapid and accurate method to identify and screen breeding materials without sample preparation is crucial for the efficiency in breeding and an acceleration of the selection process.

Considering the demands of breeding a rapeseed cultivar with high quality protein and its genetic analysis, it is necessary to develop a fast and efficient method such as near-infrared reflectance spectroscopy technology to determine amino acids composition in rapeseed meal. To date, no attempt has been made to determine amino acids content in rapeseed meal based on intact seeds by NIRS. It is for this reason that we have focused on the technology of NIRS. This work was to study the potentials of NIRS to estimate amino acid contents of rapeseed meal and to explore its applicability in identifying variability for these traits.

2. Materials and methods

2.1. Materials

An original population of 621 rapeseed samples was mainly derived from genetic experiments and the breeding programs. All seed samples including F_1 and F_2 hybrid generations and their parents were collected in the years of 2007 and 2008. Being cultivars and breeding line across environments the seed samples had a larger variation in seed qualities making them suitable for NIRS calibration. All the raw samples were scanned to collect the NIRS spectra.

2.2. Collection of spectra

WinISI II (Version1.04) software was applied to collect spectra and develop the calibration equations in this study. Whole intact rapeseed samples were scanned on a NIRSystems model 5000 monochromator (NIRSystems Inc., Silver Spring, MD, USA). Approximately 3 g of intact rapeseed samples were placed in a small ring cup of 36 mm inner diameter, and reflectance spectra ($\log 1/R$) from 1100 to 2498 nm were recorded at 2 nm wavelength increment. Each sample was subsequently scanned 32 times in small ring cells (Shenk and Westerhaus, 1993).

2.3. Selection of calibration set

A powerful approach to choose samples based on their spectra has been developed with the CENTER and SELECT algorithm by Shenk and Westerhaus (1991a). After the original population with 621 samples was scanned, the algorithm CENTER was used for the calculation of principal components and GH for the description of spectral boundaries and detection of outliers (Shenk and Westerhaus, 1991a). The number of samples reduced to 611 after outliers were excluded. Following centering of