

Classification of specialty seed meals from NIR reflectance spectra

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ABSTRACT

Near infrared reflectance spectroscopy was used to identify alternative seed meals proposed for food and feed formulations. Spectra were collected from cold pressed Camelina (*Camelina sativa*), Coriander (*Coriandrum sativum*), and Pennycress (*Thlaspi arvense*) meals. Additional spectra were collected from Dried Distillers Grains with Solubles (DDGS) which is an inexpensive co-product obtained from dry milling maize (*Zea mays*). Spectra were processed by multiplicative scatter correction and first derivative transform prior to principle component analysis (PCA). The PCA score plots showed separate groups for each material and identified potential groups for classification by linear discriminant analysis (LDA), soft independent modeling of class analogy (SIMCA), and support vector machine (SVM) methods. Results showed that LDA and SVM were both successful in classifying the type of source material while SIMCA was not able to correctly identify solvent extracted materials. The ability to rapidly and non-destructively confirm the identity and quality of components at the process line will promote the use of alternative seed meals to supplement commodity meals such as maize and soybean.

KEYWORDS: chemometrics, infrared spectroscopy, reflectance spectroscopy, specialty crops

INTRODUCTION

A diet based on corn meal and soybean meal is common in North America, however, the cost of these commodity crops has increased significantly in recent years and lower cost sources of vegetable proteins need to be developed. The implementation of infrared spectroscopic methods offers the possibility to rapidly screen ingredients, formulate blends, and measure product quality [1]. However, the deployment of the instrumentation also requires the prior development of spectral libraries or predictive models to be effective in determining the identity, purity, or product specification of the material under investigation [2]. While general-purpose instrumentation is available commercially from numerous suppliers the libraries and models required to interpret spectra need to be developed and calibrated for the specific application. Correlation equations will be developed from the spectral libraries of alternative seed meals to enable on-line measurement and prediction. Chemometric methods such as principal component analysis can be used to classify substrates and provide quality assessments of feed formulations.

Of particular interest are seed meals obtained from specialty oilseed crops. In such cases the seed oil is the high value product and the seed meal is available as an inexpensive co-product. The potential use of alternative or specialty seed meals to replace corn and soybean meals is based on both nutritional and economic factors. Consumer awareness has generated interest in food products

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with improved nutritional characteristics and enriched with functional additives. These additives include plant extracts with antioxidant or other health promoting activity. Highly unsaturated fatty acids such as docosahexaenoic acid (DHA) have attracted interest as food supplements due to reported health benefits [3, 4]. Infrared techniques have demonstrated advantages to traditional gas chromatographic methods that require expensive instrumentation, sample preparation, and long analysis times. Near infrared spectroscopy combined with chemometric methods offers a rapid and nondestructive alternative for routine food quality measurements.

Economic considerations are also significant with respect to the continuing discussion of food versus fuel where arable land may be dedicated to the production of crops for energy rather than food. However, in some cases an energy crop may provide an inexpensive food protein source as a co-product. For example, when an oilseed crop is processed for biodiesel production a defatted seed meal is also generated. This material can be an alternative or supplement to the commodity food seed meals. Other inexpensive co-products are generated during corn dry milling, e. g., dried distillers grains (DDG). This co-product is available in large quantities and has potential to supplement standard corn meal. As the use of alternative seed meals increases the need for rapid confirmation of seed meal identity and purity arises. This includes the detection of genetically modified organisms (GMO) materials that may be blended with non-GMO materials [5, 6].

Spectroscopic methods such as near-infrared spectroscopy (NIRS) are applicable to rapidly quantify the protein, fat, and moisture levels of meal products. In practice, reflectance techniques allow for rapid analysis of solid samples and may be automated with appropriate calibration. The food and feed industry is aware of this technology and is moving to adopt it although it is not currently used extensively. Infrared methods have applications at the process line in the production facility and may replace traditional analytical methods in quality control laboratories [7]. More recently portable spectroscopic instruments are combined with remote sensing technology for pre-harvest and post-harvest measurements.

MATERIALS AND METHODS

Materials

Samples of cold press camelina (CAM), cold press coriander (COR), and cold press pennycress (PC) meals; dried distillers grain (DDG); solvent extracted camelina (CAMX), hexane extracted DDG (DDGXH), and ethanol extracted DDG (DDGXE) were graciously provided by Dr. Harry O'kuru, USDA-ARS, Peoria, IL, USA.

Spectroscopy

Spectra were collected on a Perkin Elmer model 400 FTIR instrument equipped with a NIR reflectance accessory. Samples were scanned from 10,000-4,000 cm⁻¹ and a bandwidth of 2 cm⁻¹.

Chemometric analysis

Spectra were analyzed with Unscrambler version 10.1 (Camo Software, AS, Oslo, Norway). Principal component analysis (PCA) was performed with multiplicative scatter corrected spectra and first derivative spectra to identify potential groups for the development of classification schemes. Subsequent analysis was performed by linear discriminant analysis (LDA), soft independent modeling by class analogy (SIMCA), and support vector machine (SVM) classifications.

RESULTS AND DISCUSSION

The principal component analysis (PCA) scores for multiplicative scatter corrected (MSC) spectra are shown in Figure 1. Seven groups are clearly distinguishable and correspond to each of the different meals investigated. The plot displays scores for the first two principal components and accounts for 83% of the variability. The hexane extracted sample (DDGXH) shows the most dispersion. However, there is no overlap between any of the groups. These analyses were performed on the full spectra and no attempt was made to exclude particular spectral regions. It is generally possible to improve model results by iteratively modifying the input spectra with additional pre-processing steps or transformations [8-10]. Similar results were obtained when PCA was performed on first derivative spectra and in this case the first two principal components accounted for 84% of the variability (not shown). For this investigation

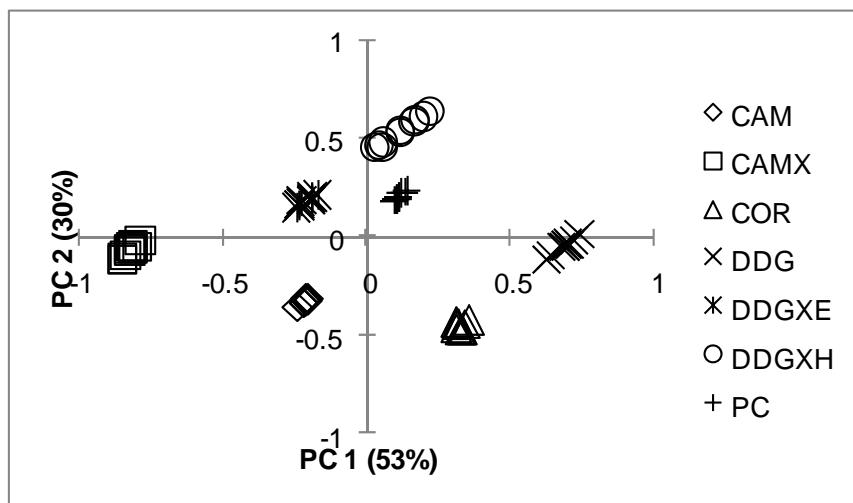


Figure 1. Score plot for principal component analysis of NIR spectra after multiplicative scatter correction.

PCA was used primarily as a guide to predict the possible success of developing a classification model. These PCA results exhibit the necessary groupings associated with the different meal substrates and provide evidence that classification methods could be successful. Additional pre-processing of the spectra was not used and the evaluation of three common classification schemes proceeded on the full spectra only with multiplicative scatter correction.

Linear discriminant analysis (LDA), soft independent modeling by class analogy (SIMCA), and support vector machine (SVM) classification models were compared using the collected spectra. LDA and SVM classification models were developed and tested on the meal samples. Both models were able to correctly classify all of the test samples with 100% success. In contrast, classification by SIMCA was effective in classifying the meal source material but not able to distinguish between extracted and non-extracted samples. Based on these results the implementation of either LDA or SVM classification methods could be used. The selection of LDA may be preferred to SVM based on the linearity of model.

CONCLUSION

Spectroscopic methods can be used to rapidly identify seed meals and is expected to facilitate the use of alternative and specialty crop co-products. Recent advancements in spectroscopic technology

enable the deployment of instrumentation for screening incoming materials and online measurements. This approach offers an economic advantage to traditional chromatographic methods. The NIR reflectance technique is a general technique applicable to carbohydrate, protein, moisture, and fat determinations with appropriate calibration. In this study the method was demonstrated for classification of substrates but could be extended for quantitative prediction of nutritional components. Raw spectra were collected, corrected, and analyzed by PCA to reveal groupings suitable for classification. These results provide the feed industry with a rapid method to classify camelina, coriander, and pennycress meals.

CONFLICT OF INTEREST STATEMENT

The authors are not aware of any conflict of interest in the publication of this original research.

REFERENCES

1. Maleki, M. R., Mouazen, A. M., Ramon, H. and de Baerdemaeker, J. 2007, Biosystems Engineering, 96(3), 427.
2. Nicola, B. M., Beullens, K., Bobelyn, E., Peirs, A., Saeys, W., Theron, K. I. and Lammertyn, J. 2007, Postharvest Biology and Technology, 46, 99.
3. Harris, W. E. 1989, Journal of Lipid Research, 30, 785.
4. Leaf, A. 1990, Circulation, 82, 624.

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5. Alishahia, A., Farahmanda, H., Prietob, N. and Cozzolinoc, D. 2010, Spectrochimica Acta Part A, 75, 1.
 6. Blanco, M. and Villarroya, I. 2002, Trends in Analytical Chemistry, 21(4), 240.
 7. le Bourse, D., Jégou, S., Conreux, A., Villaume, S. and Jeandet, P. 2010, Analytica Chimica Acta, 667, 33.
 8. Rinnan, A., van den Berg, F. and Engelsen, S. B. 2009, Trends in Analytical Chemistry, 28(10), 1201.
 9. Xiaobo, Z., Jiewen, Z., Povey, M. J. W., Holmes, M. and Hanpin, M. 2010, Analytica Chimica Acta, 667, 14.
 10. Xiaobo, Z., Jiewen, Z. and Yanxiao, L. 2007, Vibrational Spectroscopy, 44, 220.