Analysis of near infrared reflectance spectrum of rape seed with different content of erucic acid

Tamara Nosenko[1], Inna Hutsalo[1], Volodimir Nosenko[1], Irina Levchuk[2], Svitlana Litvynchuk[1]

[1]*National University of food technologies, Kyiv, Ukraine*
[2]*State Enterprise "Ukrmetrteststandard"*

Keywords:

Spectroscopy
Near–infrared
Reflectance
Rape seed,
Erucic acid

Article history:

Received 26.01.2013
Received in revised form 03.03.2013
Accepted 22.03.2013

Corresponding author:
Inna Hutsalo
E-mail:
Ksa0178@list.ua

ABSTRACT

The objective of this study was to analyze of reflectance spectrum in near-infrared region of rapeseed with different erucic acid content and to choose the most informative wavelength for development of calibration equation. Near–infrared reflectance spectra at 1330-2370 nm were measured for rape seed with high and low erucic acid content. The fatty acid composition of seed oil were determined by gas-liquid chromatography. We have detected difference in absorbance level between low and high erucic acid seed in the range of 1700-1860 and 1930-2370 nm. The first derivative of reflectance spectra were analyzed and wavelength set are proposing for development of calibration equation of erucic acid content in rape seed. Our data could be used for determination of erucic acid content in rape seed by near–infrared reflectance spectroscopy.

Introduction

Near–infrared reflectance spectroscopy (NIRS) is a widespread technique for chemical composition analysis of different agricultural seed [1,2]. The advantage of this method is nondestructive analysis without using of chemicals. It is possible to estimate moisture, protein, oil, glucosinolate content in seed by NIRS. Moreover, recently this technique was proposed to determine the fatty acid composition of seed oil, free fatty acid content and peroxide value in oil [2-5].

In order to use this technique for the measurement of some composition parameters of seed or oil development of calibration equation is necessary. For this purpose the reflectance spectra of samples with different chemical composition are measured. To receive an adequate calibration equation analysis of at least 30 samples are necessary. The more samples are using for calibration the higher reliability of equation. The even distribution of the samples within the range of calibration number of samples for the investigated parameter is important too. Reflectance data on the some wavelength range are using to calculate of calibration equation.

Additionally, development of calibration equation is necessary for the every species or at least plant family [1] and for every instrument that is being used.

On the other hand nowadays rape is a very important oil crop because of its high seed oil content and special fatty acid composition. Rape breeding was directed on the creation of rape seed with low content or without erucic acid in oil as it was shown a negative influence of this fatty acid on human and animal health. Thus now there are two groups of cultivated rape with high and low erucic acid content. The first is using for technical oil production and other one for edible oil. That is why detection of erucic acid content in rape seed is an important task for seed processing.

Although gas-liquid chromatography of fatty acid methyl esters is using for fatty acid composition determination NIRS technique is optimal for express analysis.

The objective of this study was to analyze of reflectance spectra in near-infrared region of rapeseed with different erucic acid content and to choose the most informative wavelength for development of calibration equation.

Materials and methods

Two different kind of rape seed (Brassica napus) were used, with high and low erucic acid content.

"Dry" seeds were preparing in the air oven at 105 °C bringing up their mass to the constant value.

For the reflectance spectrum measuring seed samples were grinded on the laboratory grinder.

The seed oil content was determined in milled samples by Soxhlet oil extraction with petrol ether.

For the determination of fatty acid composition seed oil was extracted on the laboratory screw press. Fatty acid composition was determined by gas-liquid chromatography of fatty acid methyl esters. They were analyzed on Hewlett Packard gas chromatograph model HP 6890 with capillary column HP-88 (88%-cyanopropyl aryl-polysiloxane, 100m x 0.25 mm x 0.25 γm film thickness (Agilent Technologies). The temperature of injector was 280 °C, detector — 290 °C. The column temperature was from 60 to 230 °C. The rate of carrier gas was 1.2 ml/min. Identification of the fatty acids was performed by comparison of the retention times with standards mixture of fatty acid methyl esters (37 Component FAME Mix, Supelco).

The reflectance spectra of samples were measured on monochromator near–infrared reflectance spectrometer Infrapid-61 model QA-262 (Hungary). For each sample the reflectance spectrum (lg 1/R) from 1330 to 2370 nm was recorded at 10-nm intervals. The first derivative from lg 1/R spectra was calculated.

Results and discussion

We have analyzed the fatty acid composition of different rape seed samples from local market. Seed moisture have shown was ranged from 8 to 10 % and fat content from 45 to 49 %. Determination of fatty acid composition detected that there were samples with low (< 5 %) and high content of erucic acid (Table 1).

We have used the samples with different content of erucic acid for the near–infrared reflectance spectra measuring. For each sample reflectance spectrum (lg 1/R) was recorded at 10 nm intervals. Obtained spectra are given on the Fig.1.

The reflectance spectra were transformed as lg 1/R (optical density) and they indicate the big difference of optical density between seed dry substances and seed with 8.5 % of moisture. The spectra of seed with actual moisture have demonstrated almost total superposition, there was only some difference in the range 1430-1630 nm and 2000-2200 nm between samples with low and high erucic acid content. Evident peaks of absorbance on the 1450 and 1930 nm wavelength are belonging to the absorbance bands of water and caused by stretching vibrations of water molecule as it is known.

Table 1. Major Fatty acids (% of total fatty acids) in rape seed oil.

Fatty acid	Mean	
	low erucic acid	high erucic acid
C 16:0	4,6	3.5
C 18:0	2,0	1.0
C18:1	50,5	13.0
C 18:2	16,9	14.0
C 18:3	7,7	9.0
C20:1	2,3	7.5
C 22:1	1,3	47.5

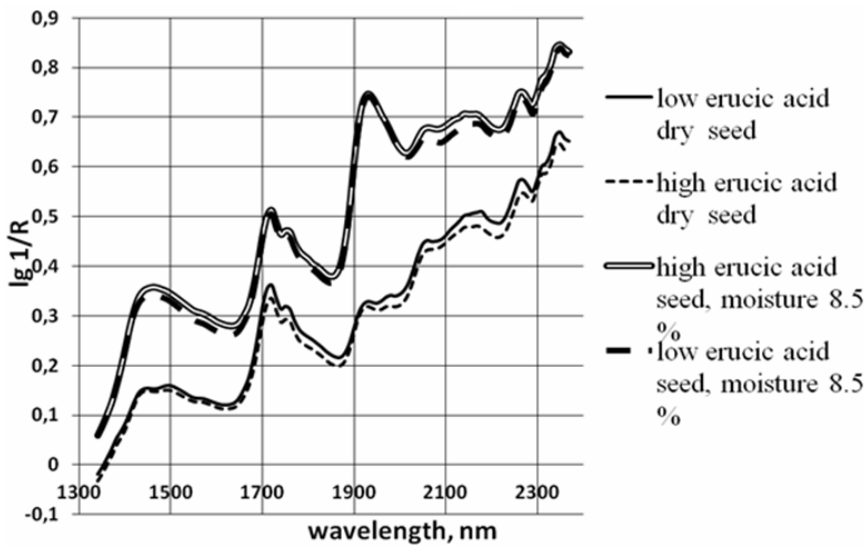

Fig.1. The reflectance spectra of low and high erucic acid rape seed.

Comparison of two spectra belonging to the "dry" seed (seed dry substances) have shown that appearance of these two spectra are very similar, but there is a difference in absorbance level between low and high erucic acid seed in range of 1700-1860 and 1930-2370 nm.

NIR spectra correspond to the highest overtones and combinations of fundamental vibrations of —CH group: the first overtone is at 1500-1800 nm and the combination bands of —CH stretching motions and deformations are at 2200-2400 nm [6]. Revealed differences in absorbance level between low and high erucic acid seed are probably explaining by these vibrations.

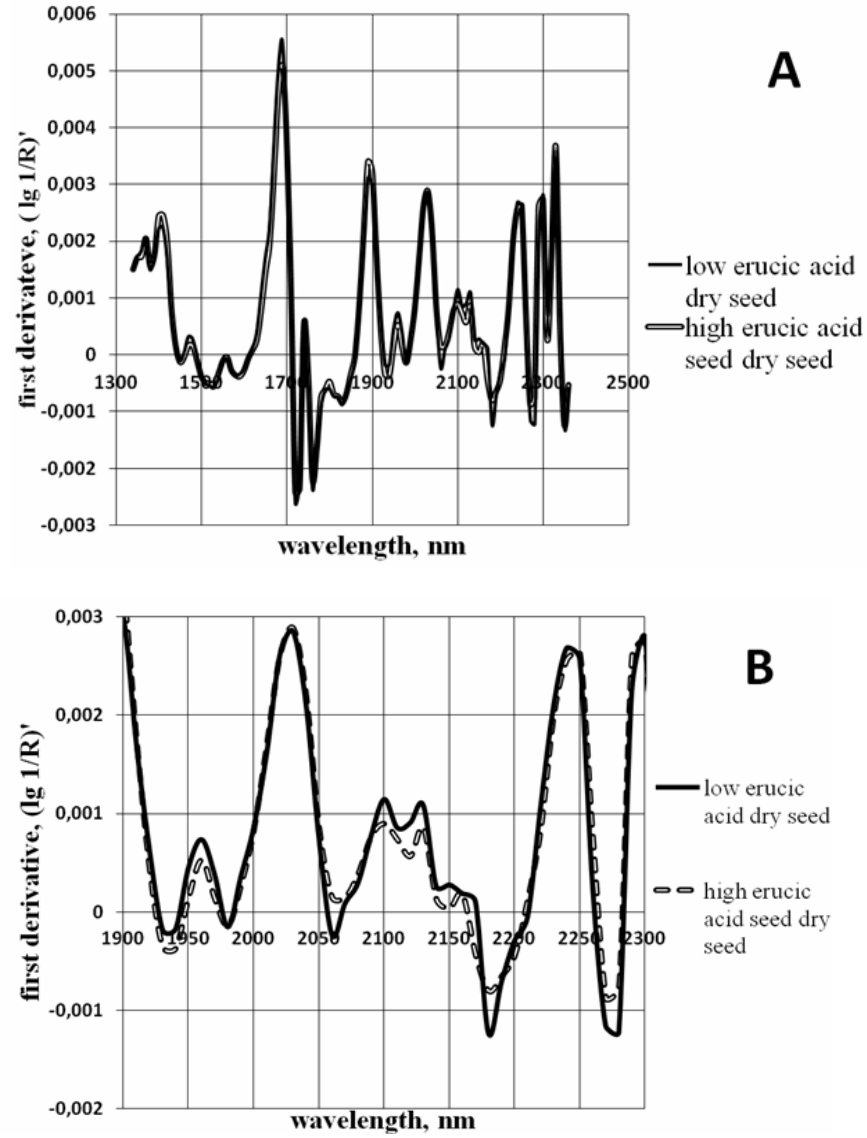

Fig.2. The first derivative of near infrared reflectance spectra of low and high erucic acid rape seed. A – at 1330-2370 nm, B – at 1920-2280 nm.

In order to get more information from absorbance spectra we have analyzed the first derivatives of these spectra (Fig.2). The most evident difference between first derivatives was detected in the range 1930-2270 nm. We suppose that they can be caused by different fatty acid composition of low and high erucic acid rape seed. We can suppose that this range is an informative for the development of fatty acid composition calibration equation.

Since at least six point of wavelength are needed for calculation programme of spectrometer Infrapid-61 we have proposed the next wavelength for the development of fatty acid composition calibration equation: 1960, 2060, 2100, 2150, 2190, 2270 nm.

Conclusions

In this study we have analyzed the reflectance spectra in near-infrared region of rapeseed with different erucic acid content which was obtained on the near–infrared reflectance spectrometer Infrapid-61. We have detected the different level of absorbance between low and high erucic acid seed at 1700-1860 and 1930-2370 nm. We have proposed some wavelength for development of calibration equation for estimation of erucic acid content in rape seed using Infrapid-61.

References

1. Velasco L., Goffman F.D., Becker H.C. Development of calibration equations to predict oil content and fatty acid composition in Brassicaceae Germplasm by Near Infrared Reflectance Spectroscopy, J. Am Oil Chem Soc, 1999,76:1, 25-30.
2. Rudolphi S., Becker H. C., Schierholt A., Witzke-Ehbrecht S., Improved Estimation of Oil, Linoleic and Oleic Acid and Seed Hull Fractions in Safflower by NIRS, J Am Oil Chem Soc, 2012, 89:363–369.
3. Moh M.H., Che Man Y.B., Voort F.R., Abdulah W.J.W., Determination of Peroxide Value in Thermally Oxidized Crude Palm Oil by Near Infrared Spectroscopy, J. Am Oil Chem Soc, 1999,76:1, 19-23.
4. Niewitetzki O, Tillmann P, Becker H.C, Mollers C., A new near-infrared reflectance spectroscopy method for high-throughput analysis of oleic acid and linolenic acid content of single seeds in oilseed rape (Brassica napus L.), J Agric Food Chem, 2010, 58, 94–100.
5. Azizian H., Kramer J. K. G., Mossoba M. M., Evaluating the Transferability of FT-NIR Calibration Models for Fatty Acid Determination of Edible Fats and Oils Among Five Same-make Spectrometers Using Transmission or Transflection Modes with Different Pathlengths, J Am Oil Chem Soc, 2012, 89:2143–2154.
6. Shenk, J.S., J.J.Workman, Jr., M. Westerhaus, Application of NIR Spectroscopy to Agricultural Products, in Handbook of Near-Infrared Analysis, edited by D.A. Burns and E.W. Ciurczak, Marcel Dekker, Inc., New York, 1990, pp.383-431.
7. Wai Lam Yip, Ingvil Gausemel, Sverre Arne Sande, Knut Dyrstad. Strategies for multivariate modeling of moisture content in freeze-dried mannitol-containing products by near-infrared spectroscopy / Journal of Pharmaceutical and Biomedical Analysis, Volume 70, November 2012, Pages 202-211
8. Craig M. Gardner, Huwei Tan, Edward L. Hull, Jennifer B. Lisauskas, Stephen T. Sum, Thomas M. Meese, Chunsheng Jiang, Sean P. Madden, Jay D. Caplan, Allen P. Burke, Renu Virmani, James Goldstein, James E. Muller. Detection of Lipid Core

Coronary Plaques in Autopsy Specimens With a Novel Catheter-Based Near-Infrared Spectroscopy System / JACC: Cardiovascular Imaging, Volume 1, Issue 5, September 2008, Pages 638-648

9. Valentina Quaresima, Silvia Bisconti, Marco Ferrari. A brief review on the use of functional near-infrared spectroscopy (fNIRS) for language imaging studies in human newborns and adults / Brain and Language, Volume 121, Issue 2, May 2012, Pages 79-89
10. D.K. Lovett, E.R. Deaville, D.I. Givens, M. Finlay, E. Owen. Near infrared reflectance spectroscopy (NIRS) to predict biological parameters of maize silage: effects of particle comminution, oven drying temperature and the presence of residual moisture / Animal Feed Science and Technology, Volume 120, Issues 3–4, 28 May 2005, Pages 323-332
11. T. Shimokawa, K. Suzuki, T. Misawa, K. Miyagawa. Predictability of investment behavior from brain information measured by functional near-infrared spectroscopy: A bayesian neural network model / Neuroscience, Volume 161, Issue 2, 30 June 2009, Pages 347-358