Development of Near-Infrared Reflectance Spectroscopy to Estimate Oil Content in Safflower

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Summary

The oil of safflower (*Carthamus tinctorius* L.) is a valuable oil for human nutrition. It contains a high amount of unsaturated fatty acids, in particular linoleic acid (up to 90 %). There is a great demand for ecologically produced oil in Germany, though oil crops are cultivated on 2 % of the ecological acreage.

In Germany, hardly any variety test exists, moreover there has been no breeding efforts so far, although genetic variation in safflower is large. The aim of this study was the development of a rapid and non-destructive method to determine oil content in safflower seed using NIRS (Near-Infrared Reflectance Spectroscopy).

A total of 203 seed samples were scanned with NIRS to estimate the oil content. Intact seeds as well as milled seeds were tested. The reference values for calibration were obtained with the Soxhlet extraction technique.

The oil content analysed by Soxhlet ranged from 10% to 29.6%. NIRS-scanning of milled seed showed better values of calibration compared to intact seed (milled seed: coefficient of determination of calibration: RSQ=0.96, coefficient of determination of cross validation: 1-VR=0.93; intact seed RSQ=0.90, 1-VR=0.82).

These results show that NIRS appears to be a suitable, rapid method to estimate oil content in safflower.

Introduction

In Germany oil crops are cultivated on 2% of the ecological acreage only while there is a great demand for ecologically produced oil. Safflower yields a valuable oil for human nutrition. It shows the highest ratios of polyunsaturated/-saturated fatty acids of any available oil and high levels of linoleic or oleic acid (Li Dajue and Mündel 1996).

The genetic variation of safflower is large, but hardly any variety test exists in Germany so far and there has been also no breeding in progress. The determination of seed quality like oil content with chemical methods is very laborious. A reliable estimation of seed weight, oil content, oleic and erucic acid in intact, single seeds of rapeseed is possible by using the NIRS-technique (Velasco et al. 1998, Velasco et al. 1999). Furthermore good results were achieved for estimating the content of moisture, oil and protein in sunflower (Moschner et al. 2004). The development of a rapid, precise, non-destructive and reasonable method to evaluate quality components in safflower is of major interest to growers, processors and breeders alike.

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Materials and Methods

In 2002, a total of 741 safflower accessions from different genebanks throughout the world was grown in a replicated trial in two locations in Germany (Stuttgart and Göttingen). The overall objective of this research was to evaluate agro-morphological traits as well as fatty acid composition. In the following year, 65 genotypes were tested in a replicated trial at the same locations. Moreover first crosses have been done in 2002. In 2004, 250 F2-progenies were cultivated in Göttingen in single rows. Different seed samples of these years were taken to develop the first NIRS calibration.

About 3-5 g seeds of each of 95 genotypes cultivated in 2003 were scanned with NIR Systems model 6500 monochromator instrument (NIR Systems, Inc., Silver Spring, MD). Intact seeds (achenes) as well as milled seeds were tested. They were placed in a small ring cup (i.d. 4.7 cm). Reflectance spectra (log1/R) were collected between 408 and 2492.8 nm. Additionally, 108 samples of 2004 were analysed. The measurement of the intact seed was replicated three times and averaged.

The oil content of these 108 and 95 samples was analyzed by the Soxhlet oil extraction technique. Oil was extracted from 500 mg seed flour of each sample by petrol ether for about 8 hours.

Results of these analyses were used to develop the NIRS-calibration by using of WinISI II version 1.50 (Infrasoft International, Hosham, West Sussex, United Kingdom) software. NIRS spectra were matched with reference data and the calibration was calculated by using modified partial least square (MPLS) regression and math treatment 1, 4, 4, 1.

Results and Discussion

The oil content analysed by Soxhlet ranged in 2003 from 17.5% to 29.6% and in 2004 from 10% to 29.6%.

The calibration statistics for oil content analysed in intact seed and milled seed are shown in table 1. The coefficient of determination of calibration and coefficient of determination of cross validation are higher in the equation for scanning milled seed (milled seed 95 samples: RSQ=0.91, 1-VR=0.83; milled seed 108 samples: RSQ=0.92, 1-VR=0.91; milled seed all samples RSQ=0.96, 1-VR=0.93). Furthermore the standard error and the standard error of cross validation are lower (milled seed 95 samples: SEC= 0.66, SECV=0.90; milled seed 108 samples: SEC=1.01, SECV=1.09; milled seed all samples SEC= 0.77, SECV=0.99). This may be caused by the thickness of the hull. Pazdernik et al. (1997) reported that calibration equations based on ground soybean samples were more accurate than those based on intact seed samples, which might be explained by diversity of surface area and size of the seeds used. It may be possible that the chemical information is obscured by changes in the spectra caused by differences in seed size and shape (Baye and Becker 2004). Further the variation of oil content is higher for the 108 samples from 2004

Table 1: Calibration and cross validation statistics in NIRS equations for the analysis of oil content in intact seed and milled seed

	Calibration							Cross validation	
	N	Mean	Min	Max	SD	RSQ	SEC	1-VR	SECV
Intact seed (2003)	95	24.48	17.5%	29.6%	2.16	0.82	0.92	0.76	1.07
Milled seed (2003)	95	24.48	17.5%	29.6%	2.16	0.91	0.66	0.83	0.90
Intact seed (2004)	108	20.41	10%	29.6%	3.61	0.91	1.09	0.81	1.58
Milled seed (2004)	108	20.41	10%	29.6%	3.61	0.92	1.01	0.91	1.09
Intact seed (all)	203	22.31	10%	29.6%	3.64	0.90	1.16	0.82	1.53
Milled seed (all)	203	22.31	10%	29.6%	3.64	0.96	0.77	0.93	0.99

N: number of samples; RSQ: coefficient of determination of calibration; SEC: SE of calibration; 1-VR: coefficient of determination of cross validation; SECV: SE of cross validation

Figure 1 and 2 show the scatter plots of predicted versus measured values for intact and milled seed. The reference values for samples of 2004 are spread more widely in contrast to the samples of 2003 (see table 1). The reference values show a relatively good relationship to the NIRS values. In all cases correlation is lower on the basis of intact seed samples.

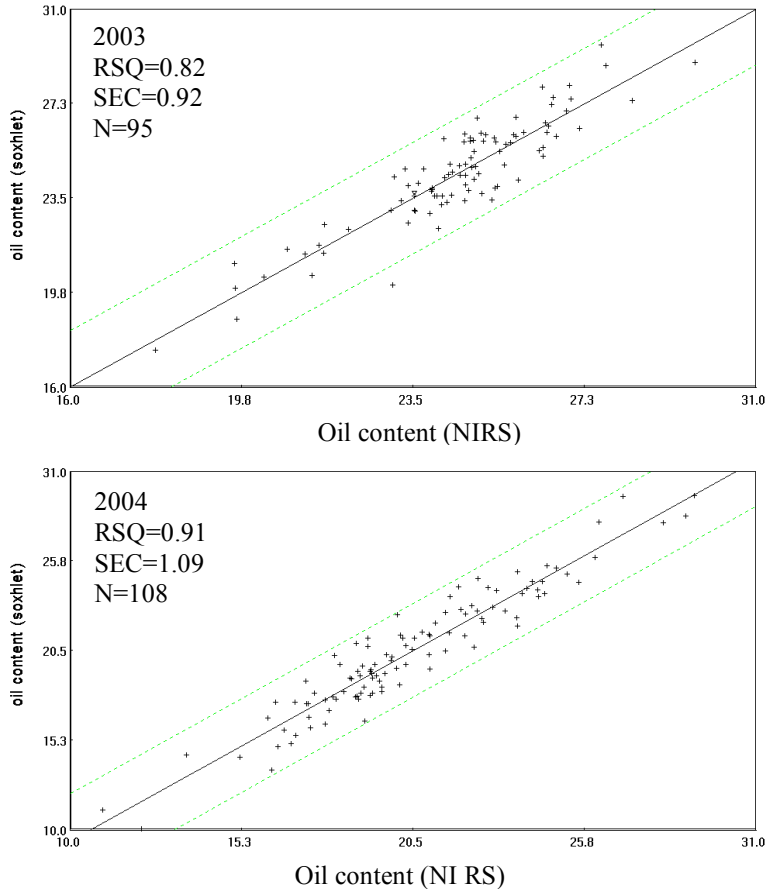

Figure 1: Reference versus NIRS-predicted values in intact seed

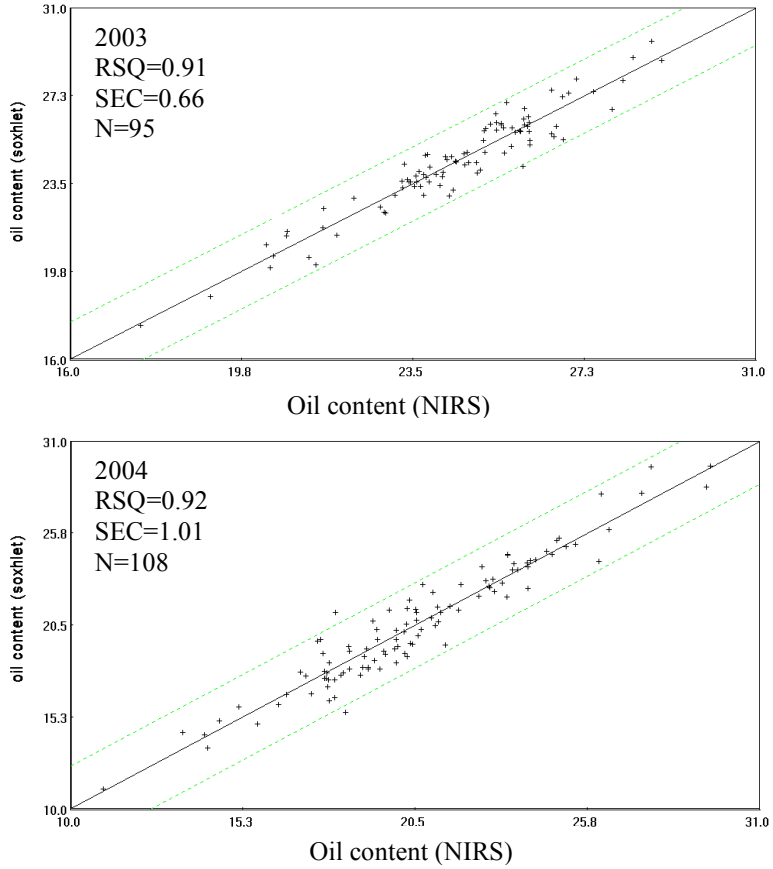

Figure 2: Reference versus NIRS-predicted values in milled seed

Conclusion

NIRS as an early screening technique is extremely useful for predicting oil content, as this is the most difficult trait in terms of time and sample size requirements in conventional chemical analysis (Baye and Becker 2004). In this study the results of the calibration show that NIRS is a suitable method to estimate oil content in safflower. The coefficient of determination of calibration and the coefficient of determination of cross validation are high especially if seed samples were milled prior to NIRS scanning (RSQ=0.96, 1-VR= 0.93).

Estimating oil content by scanning intact seed would be preferable for evaluating small seed samples. Future research should aim to improve the accuracy of the prediction by adding a broader range of samples to the calibration set.

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