Estimating the quality-parameters of ground and intact sunflower seeds by near-infrared spectroscopy (NIRS)

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Abstract

A reliable recording of the different qualities of sunflowers in order to realise an optimum of utilisation in food and non food area is necessary. For this aim it will be a benefit to use NIRS for the estimation of fatty-acid content and other quality parameters. Our aim was to create NIRS calibrations for ground and intact achenes which determine simultaneously the important quality parameters of sunflower seeds with adequate exactness and which is more time- and cost-saving than the conventional reference analysis. Available for the calibration development were different types of sunflower seed samples and two spectrometers of the type NIRSystems 6500. We achieved good results for estimating the content of moisture, oil and protein as well as the main fatty-acids. Further development of the methods is the aim of our next investigations. Apart from the extension of the database and inclusion of further parameters, e.g. free fatty acids content, cross-linkings of the calibration-equations will be worked out. All this leads to a large utility for the group of people, which is concerned with cultivation, marketing and breeding of sunflowers.

Media summary

We achieved good results for estimating the content of moisture, oil and protein as well as the main fattyacids of ground and intact sunflower seeds by use of near-infrared-spectroscopy (NIRS).

Key Words

Sunflower, NIRS, ground and intact achenes, protein, oil, fatty acids

Introduction

Supplementary to the stabilisation of the certainty of yield of high-oleic sunflowers in Germany a reliable recording of the different qualities of sunflowers in order to realise an optimum of utilisation in food and non food area is necessary. Contrary to the incoming goods inspection early selection decisions in sunflower breeding require a secured quality determination of only little sample quantities.

For this aim it will be a benefit to use NIRS after successful calibration for the estimation of fatty-acid content and other quality parameters. The advantages of NIRS are the enormous speed as well as the simple and simultaneous dertermination of many parameters (P?rez-Vich *et al.* 1998, Moschner 2003).

It is generally usual to use intact seeds in the NIRS-analysis of grain and rapeseed to achieve a non destructive measurement, whereas the measurement of intact achenes of sunflower is less satisfying due to the morphology and in particular the thickness of the pericarps (Biskupek-Korell *et al.* 2004, Velasco *et al.* 2004).

The aim of our previous investigations was to create NIRS calibrations for ground and intact achenes which determine simultaneously the important quality parameters of sunflower seeds with adequate exactness and which is more time- and cost-saving than the conventional reference analysis.

Materials and methods

For the development of the NIRS calibrations we had a large sample base at our disposal. Both ground and intact achenes were measured by near-infrared-spectroscopy. Two spectrometers of the type NIRSystems 6500 of the company *FOSS* were used, which differed only in the system of the sample presentation. In case of the measurement of intact seeds approximately 150 g were needed for filling the cuvette. Only 2 g would be enough to collect spectra from the ground material, but in this case 20 g seeds were required for the homogenous grinding. The important impact of grinding is to get a fine-grained, pourable and homogenous grist in which the pericarp is also micro-milled. The fineness of the meal increases by the time of milling but, on the other hand, too long milling leads to the destruction of the oil bodies as well as an increasing of temperature of the sample so it forms conglomerates, which cannot be eliminated by following mixing. Therefore it is very important for the achievement of reproducible results to use an uniform grinding protocol (Biskupek-Korell *et al.* 2004).

For the calibration development the sample parameters were analysed by reference methods: Content of moisture (drying oven, 105?C), protein (nitrogen determination, DUMAS), oil (NMR), fatty acids (GC).

The calibration equations for both variants (ground and intact seeds) were performed with WinISI II software (Infrasoft International). The original spectra, log (1/R), were corrected by using 2^{nd} derivative transformation (2,10,10,1), MPLS-method and SNV / detrend scatter correction. The range of wavelengths was limited to 1100 - 2500 nm, which leads to better results (P?rez-Vich *et al.* 1998). Both sample sets for calibration and validation of the variants "ground achenes" and "intact achenes" consisted of an identical sample base to enable a proper comparison of both methods.

Results

In the present study the results obtained demonstrate well the suitability of the NIRS methods for the estimation the quality parameters of ground and intact sunflower achenes, e.g. content of oleic and stearic acid. The fast and simultaneous determination of several parameters as well as the reduction of time for sample preparation are further advantages of these methods. In the following table the NIRS results for estimating the content of protein, oil, oleic and stearic acid are specified.

Table 1: Results and statistical parameters of validation "Intact achenes" vs. "Ground achenes", NIRSystems 6500, MPLS-method (Moschner?2003)

?	"Intact achenes"			"Ground achenes"		
Parameter	SEP ¹	SEP(C) ²	R ²³	SEP	SEP(C)	R^2
Protein	0,72	0,74	0,77	0,34	0,35	0,95
Oil	0,68	0,67	0,83	0,62	0,64	0,90
Oleic acid	0,96	0,99	0,81	0,52	0,54	0,94

Stearic acid	0,22	0,22	0,94	0,17	0,17	0,95
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¹ SEP [standard error of prediction] is calculated as standard deviation of all NIRS values in relation to the reference values of the validation-samples

²SEP(C) [standard error of prediction corrected for bias]

³ R^{2 is} the coefficient of determination. The closer this value is to 1, the stronger is the relationship between the reference values and the NIRS values.

Obviously the estimation of the quality parameters of intact achenes is not as exact as the results for ground achenes; however the exacteness os estimation is sufficient for many applications, e.g. for selection decisions in breeding programs, and comprises some advantages: Apart from the substantial reduction of work through omission of grinding and cleaning the cuvettes it enables breeders to consider several parameters for the selection decisions and to use the same material after the nondestructive measurement.

Conclusion

Further development of the methods is the aim of our next investigations. For an efficient use of the "intact achenes" method in practical breeding we will examine to what extent the sample quantity concerning one cuvette can be reduced in order to obtain reliable predictions. This could be a benefit for breeders, if only small amounts of the breeding material are available. In order to achieve robust calibrations and to increase the exactness of the prediction for all parameters we have large sample quantities from a triennial field test at the FAL, Braunschweig, Germany, for the extension of the database at our disposal. Apart from the inclusion of further parameters, e.g. free fatty acids content, cross-linkings of the calibration-equations will be worked out. All this leads to a large utility for the group of people, which is concerned with cultivation, marketing and breeding of sunflowers.

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References

Biskupek-Korell,?B.; Rauscher,?P.; Eidner,?S., 2004: Entwicklung einer NIRS-Kalibration zur Bestimmung des ?ls?uregehalts an vermahlener Sonnenblumensaat als qualit?tssichernde Ma?nahme bei Vermarktung und Verarbeitung von High-Oleic-Sonnenblumen. In: UFOP-Schriften, Jg.?2004, in Vorbereitung

Moschner,?C.?R,?2003: Absch?tzung des Gehaltes wertgebender Inhaltsstoffe von Sonnenblumensaat mittels Nahinfrarotspektroskopie.

(http://www.fh-hannover.de/imperia/md/content/zentral/forschung/berichte/nirs-diplom.pdf)

P?rez-Vich, B.; Velasco, L.; Fern?ndez-Mart?nez, J. M., 1998: Determination of seed oil content and fatty acid composition in sunflower through the analysis of intact seeds, husked seeds, meals and oil by near-infrared reflectance spectroscopy. In: J. Am. Oil Chem Soc., 75.?Jg., H.?5, S.?547-555.

Velasco, L.; P?rez-Vich, B.; Fern?ndez-Mart?nez, J.M., 2004: Use of Near-Infrared Reflectance Spectroscopy for Selecting for High Stearic Acid Concentration in Single Husked Achenes of Sunflower . In: Crop Sci.,?Jg. 2004, H.?44, S.?93-97