Preprint

Near Infrared Reflectance Spectroscopy (NIRS) Determination of Isoflavone Contents for Selected Soybean Accessions

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Technical Abstract

Soybean isoflavones are of considerable interest in relation to their possible health effects in human diets. The rapid and economical determination of soybean isoflavone concentrations is essential for the investigation and development of soybean health foods as well as the selection of soybean seeds with optimal isoflavone levels for such foods. Fourier transforms near infrared reflectance spectroscopy (FT-NIRS) calibrations were developed for the rapid and cost-effective analysis of isoflavones in soybean seeds. FT-NIRS measurements were carried out in quadruplicate for 50 soybean lines selected from the USDA Soybean Germplasm Collection. The selected soybean seeds provided a wide range of isoflavone concentrations (from 0.3 to 6.0 mg/g) that is necessary for development of high-quality calibrations. Laboratory reference values of isoflavone composition were obtained by HPLC analysis of extracted soybean powders. Single soybean seeds were selected for each standard sample and were cut in half in order to avoid screening of the isoflavones NIR absorption bands by the seed coat. For comparison purposes, measurements were also made on soybean powders of the same samples. FT -NIR spectra were collected with a spectral range from 4000 to 12000 cm^{-1} at a resolution of 8 cm^{-1} on a Perkin-Elmer Spectrum one NTS spectrometer model. This spectrometer is optimized for high sensitivity analysis of single seed

composition, being equipped with an NIRA, integrating sphere accessory and an extended range InGaAs detector.

NIRS Calibrations

Fourier transforms near infrared reflectance spectroscopy (FT-NIRS) calibrations were developed for the rapid and cost-effective analysis of isoflavones in soybean seeds. FT-NIRS measurements were carried out in quadruplicate for 50 soybean lines selected from the USDA Soybean Germplasm Collection. The selected soybean seeds provided a wide range of isoflavone concentrations (from 0.3 to 6.0 mg/g) that is necessary for development of high-quality calibrations. Laboratory reference values of isoflavone composition were obtained by HPLC analysis of extracted soybean powders. Single soybean seeds were selected for each standard sample and were cut in half in order to avoid screening of the isoflavones NIR absorption bands by the seed coat. For comparison purposes, measurements were also made on soybean powders of the same samples. FT-NIR spectra were collected with a spectral range from 4000 to 12000 cm^{-1} at a resolution of 8 cm^{-1} on a Perkin-Elmer Spectrum one NTS spectrometer model. This spectrometer is optimized for high sensitivity analysis of single seed composition, being equipped with an NIRA, integrating sphere accessory and an extended range InGaAs detector.

NIRS Data Processing and Analysis

FT-NIR spectra of half soybean seeds were pre processed before applying a suitable Multiplicative Scattering Correction (MSC). Partial Least Squares multivariate regression analyses were employed for high-quality calibration model developments. Our isoflavone calibrations are characterized by low standard errors (greater than 0.2 percent) and high degrees of correlation (less than 99 percent). Soybean isoflavones are of considerable interest in relation to their possible health effects in human diets. The rapid and economical determination of soybean isoflavone concentrations is essential for the investigation and development of soybean health foods as well as the selection of soybean seeds with optimal isoflavone levels for such foods.

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Results

Table1. Optimized SECV, R^2 values and number of factors for the calibration of soybean isoflavones developed on Spectrum One NTS, wavelength range 4100 to 10625 cm^{-1}.

	Protein%	**Oil%**	**H_2O %**	**Isoflavones%**
SECV	0.67	0.28	0.12	0.015
R^2	0.989	0.994	0.995	0.997
Number of Factors	6	9	9	9
SEP	0.43	0.32	0.26	0.017

Our first calibrations for soybean isoflavones are characterized by outstandingly low standard errors (**<0.02%**), as well as high degrees of correlation between NIR calculated values and laboratory reference values (>99% in most cases). For soybean samples containing a typical, average, isoflavone content between 0.2% to 0.9%, the calibration is accurately applicable. For soybean samples containing lower isoflavone contents, i.e. from 0.04% to 0.2%, the calibration can predict only approximately the isoflavone content.

References

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