Determination of Isoflavone Contents for Selected Soybean Lines by Fourier Transform Near Infrared Reflectance Spectroscopy

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Abstract

- Soybean isoflavones are of considerable interest in relation to their possible health effects in human diets. Rapid and economical determination of soybean isoflavone contents is essential for breeding and selection of soybean seeds with optimal isoflavone levels

- Fourier Transform Near Infrared Spectroscopy (FT-NIR) calibrations were developed for rapid and reliable analysis of soybean isoflavone content. Our isoflavone calibrations are characterized by low standard errors (<0.02%) and high degrees of correlation (>99%).

Introduction

- Soybean isoflavones are the phytochemical constituents of soybean seeds. The major isoflavones in soybeans are genistein and daidzein, and their metabolites.

- Near Infrared (NIR) spectroscopy has been applied to the rapid analysis of major soybean components such as protein and oil. State-of-the-art FT-NIR instruments have significantly improved sensitivity and therefore have the potential for analysis of low-level components such as isoflavones. In our study, a state-of-the-art FT-NIR instrument was calibrated for soybean isoflavone analysis.

NIR Instrument

- Bruker's Vector-22 FT-NIR Spectrometer
  - Detector: Integrating sphere with PbSe
  - Spectral Range: 12,000 ~ 4,000 cm^{-1}

Selection of Standard Soybean Samples

Selection of Standard Soybean Samples

Acquisition of Soybean NIR Spectra for Isoflavone Analyses

- Most of the soybean standard samples that were selected for analyses had black, or brown, seed coat. In order to avoid the interference from the pigments in the seed coat, soybean seeds were cut in half prior to acquiring spectra, and the half seed's flat sides were measured. For comparison purposes, soybean seeds were also ground and soybean powder spectra were collected.

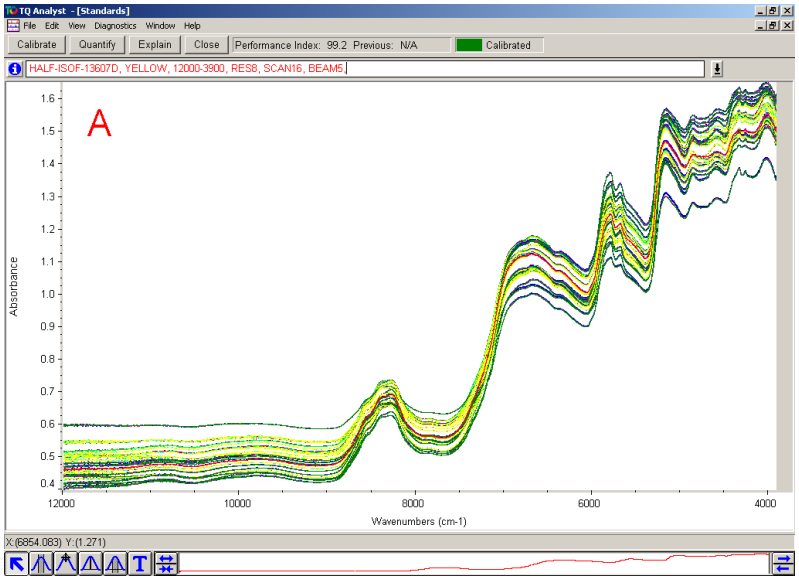
- NIR spectra were collected for each soybean sample in the spectral range between 12,000 and 4,000 cm^{-1} with a resolution of 8 cm^{-1} on a Bruker Vector-22 spectrometer.

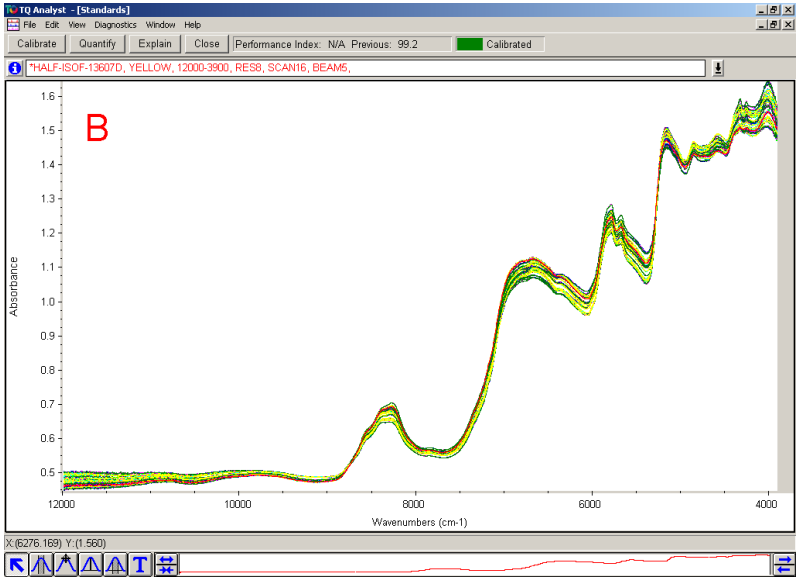
Spectra Preprocessing and Calibration Development

- Prior to calibration development, FT-NIR spectra of soybean standards were corrected for baseline variations and light scattering effects with baseline correction, normalization, and Multiplicative Scattering Correction (MSC).

- Calibrations for the total isoflavone content, protein, oil, and moisture were then developed based on the Partial Least Squares, Type 1 (PLS-1) model.

Overlay Plot of FT-NIRS Spectra of Soybean **Half Seed** Obtained with the Bruker Vector-22 FT-NIR Instrument.

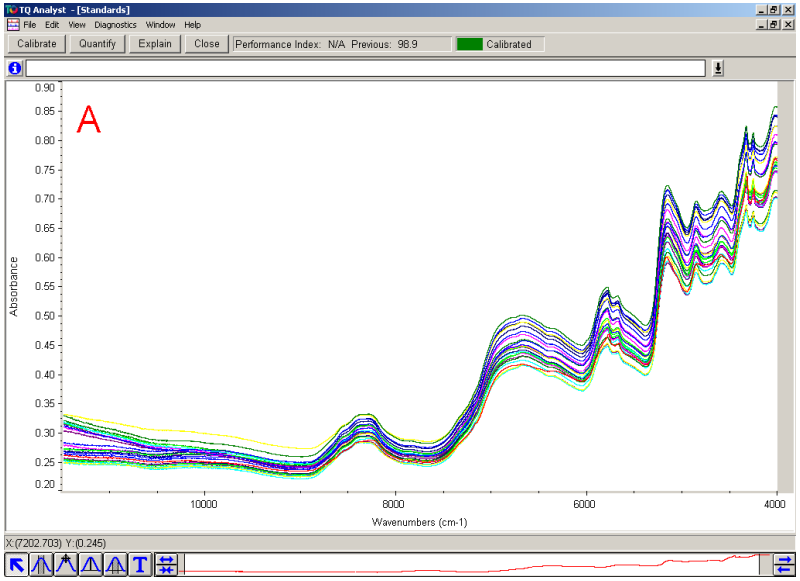


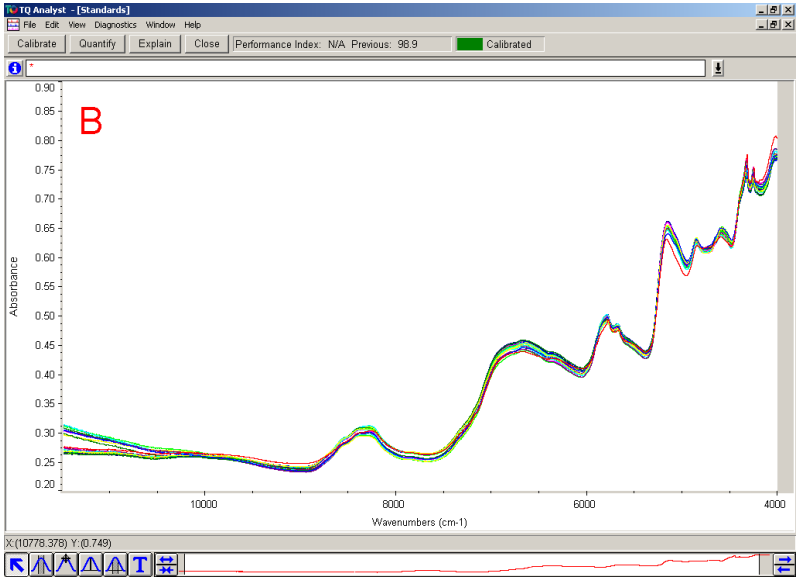


A: Raw, NIR spectra

B: After Multiplicative Scattering Correction (MSC)

Overlay Plot of FT-NIRS Spectra of Soybean **Powder** Obtained with the Bruker Vector-22 FT-NIR Instrument.





A: Raw, NIR spectra

B: After Multiplicative Scattering Correction (MSC)

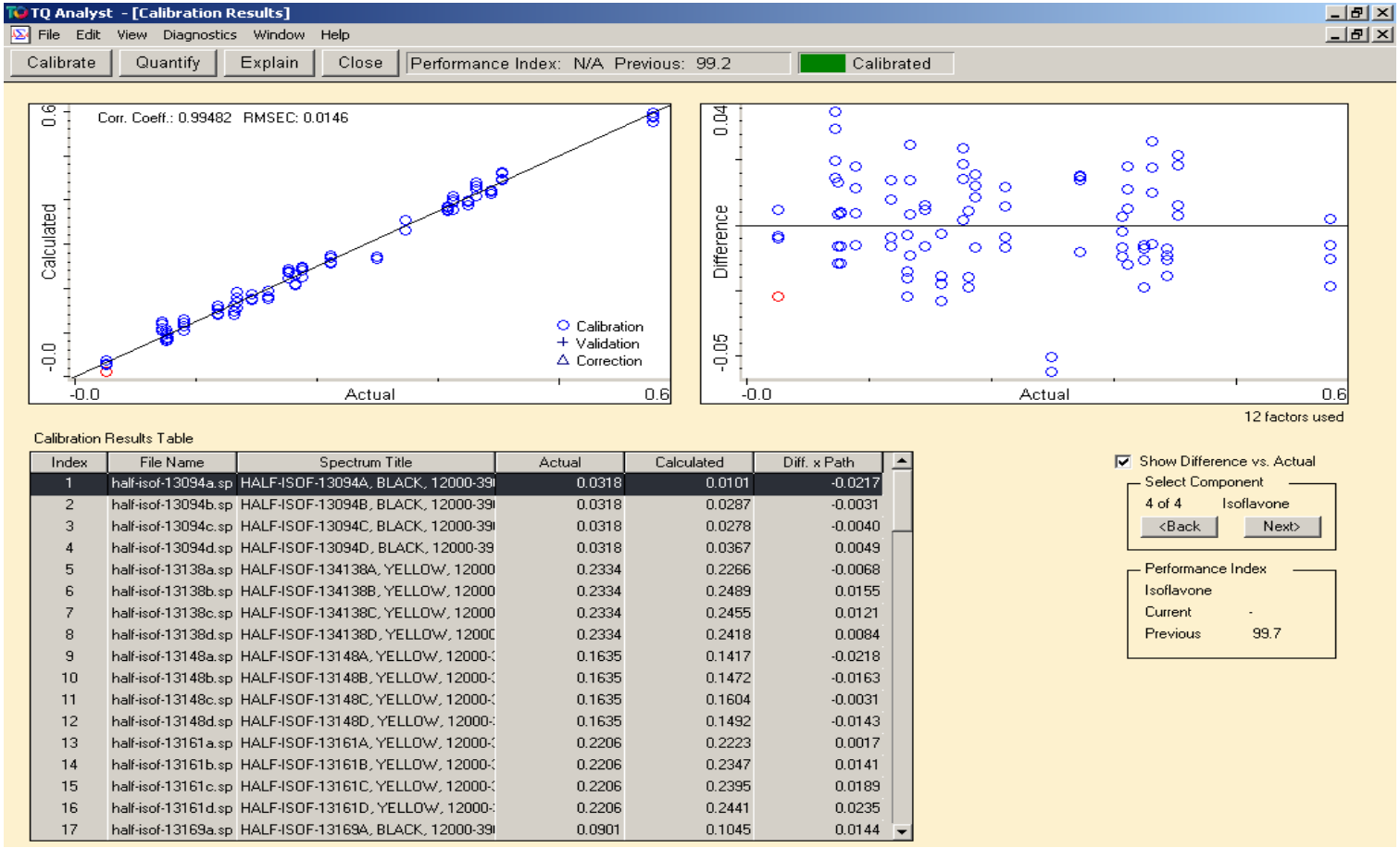
Correlation Coefficients (R) and Standard Error of Cross Validation (SECV) for the Soybean **Half Seed** Calibration Obtained with the Bruker Vector-22 Instrument

Component	Number of Factors	R	SECV
Total Isoflavones	12	99.5%	0.015
Protein	12	99.8%	0.16
Oil	12	99.8%	0.10
Moisture	12	99.7%	0.05

Correlation Coefficients (R) and Standard Error of Cross Validation (SECV) for the Soybean **Powder** Calibration Obtained with the Bruker Vector-22 Instrument

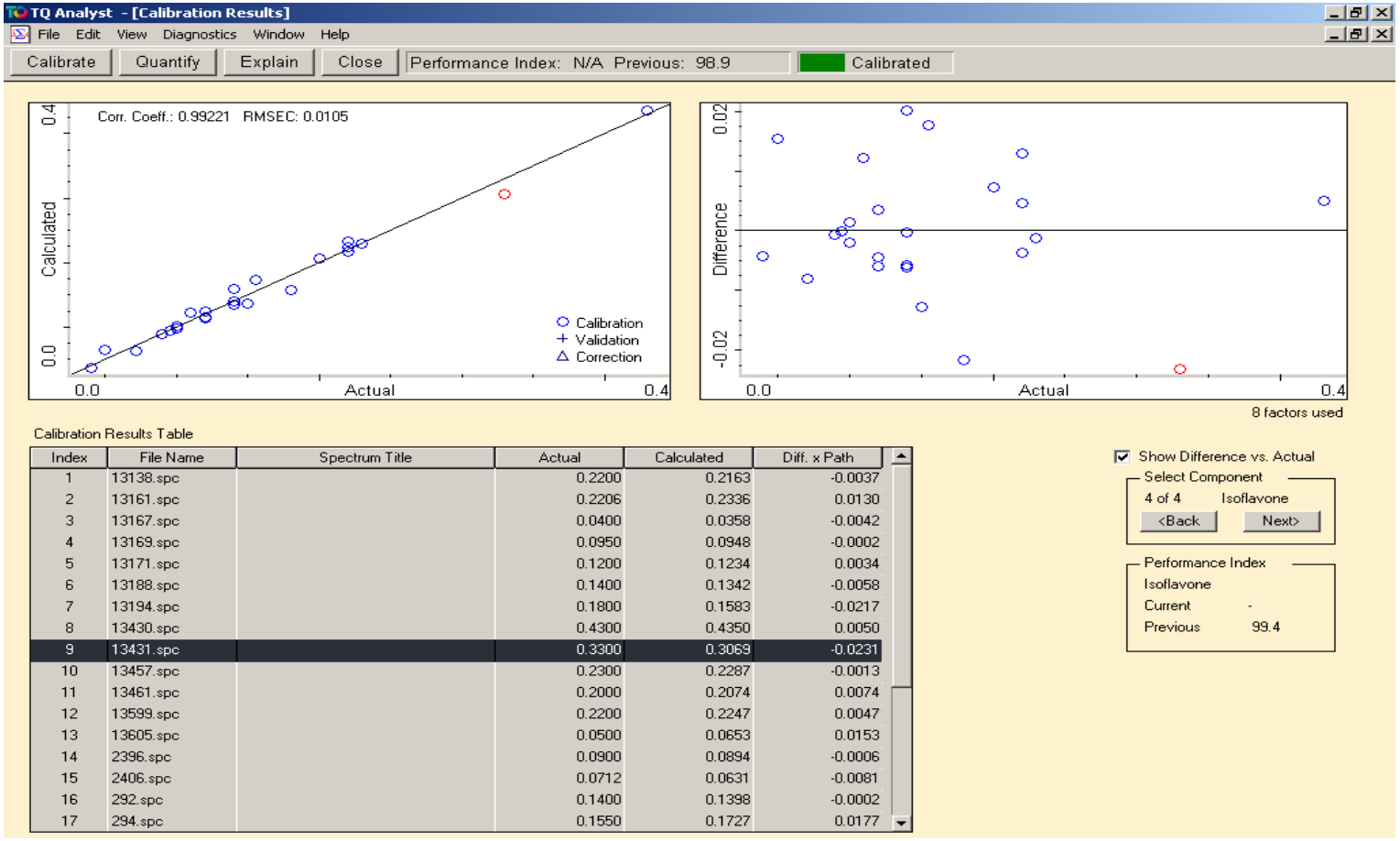
Component	Number of Factors	R	SECV
Total Isoflavones	8	99.2%	0.011
Protein	9	99.7%	0.24
Oil	8	99.8%	0.14
Moisture	8	99.9%	0.05

NIR Predicted vs Reference Values of Total Isoflavone Content (**Half Soybean Seed** Calibration Obtained with the Bruker Vector-22)



Index	File Name	Spectrum Title	Actual	Calculated	Diff. x Path
1	half-isof-13094a.sp	HALF-ISOF-13094A, BLACK, 12000-39	0.0318	0.0101	-0.0217
2	half-isof-13094b.sp	HALF-ISOF-13094B, BLACK, 12000-39	0.0318	0.0287	-0.0031
3	half-isof-13094c.sp	HALF-ISOF-13094C, BLACK, 12000-39	0.0318	0.0278	-0.0040
4	half-isof-13094d.sp	HALF-ISOF-13094D, BLACK, 12000-39	0.0318	0.0367	0.0049
5	half-isof-13138a.sp	HALF-ISOF-134138A, YELLOW, 12000	0.2334	0.2266	-0.0068
6	half-isof-13138b.sp	HALF-ISOF-134138B, YELLOW, 12000	0.2334	0.2489	0.0155
7	half-isof-13138c.sp	HALF-ISOF-134138C, YELLOW, 12000	0.2334	0.2455	0.0121
8	half-isof-13138d.sp	HALF-ISOF-134138D, YELLOW, 12000	0.2334	0.2418	0.0084
9	half-isof-13148a.sp	HALF-ISOF-13148A, YELLOW, 12000-	0.1635	0.1417	-0.0218
10	half-isof-13148b.sp	HALF-ISOF-13148B, YELLOW, 12000-	0.1635	0.1472	-0.0163
11	half-isof-13148c.sp	HALF-ISOF-13148C, YELLOW, 12000-	0.1635	0.1604	-0.0031
12	half-isof-13148d.sp	HALF-ISOF-13148D, YELLOW, 12000-	0.1635	0.1492	-0.0143
13	half-isof-13161a.sp	HALF-ISOF-13161A, YELLOW, 12000-	0.2206	0.2223	0.0017
14	half-isof-13161b.sp	HALF-ISOF-13161B, YELLOW, 12000-	0.2206	0.2347	0.0141
15	half-isof-13161c.sp	HALF-ISOF-13161C, YELLOW, 12000-	0.2206	0.2395	0.0189
16	half-isof-13161d.sp	HALF-ISOF-13161D, YELLOW, 12000-	0.2206	0.2441	0.0235
17	half-isof-13169a.sp	HALF-ISOF-13169A, BLACK, 12000-39	0.0901	0.1045	0.0144

NIR Predicted vs Reference Values of Total Isoflavone Content (**Soybean Powder** Calibration Obtained with the Bruker Vector-22)



Discussion and Conclusions

- NIR calibrations were successfully developed for determination of soybean isoflavone contents in half soybean seeds and powders
- The Multiplicative Scattering Correction (MSC) significantly reduces spectral variations that are not related to concentration changes, thereby improving the reliability of isoflavone calibrations.
- Our isoflavone calibrations for both soybean half seeds and powders are characterized by low standard errors (<0.02%) and high degree of correlation (>99%).

Acknowledgements

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