Application Note – N°. 903/2025

On-site soybean quality analysis with proxiScout™

Abstract: The following study evaluates the ProxiScout™ handheld NIRS analyzer for rapidly and non-destructively predicting oleic and linoleic acid content in soybeans. Differentiating high-oleic soybeans from conventional ones is crucial for ensuring product quality, meeting labeling requirements, and maximizing value in the supply chain.

BÜCHI

1. Introduction

As the demand for high-oleic soybean oil increases due to regulatory restrictions on trans-fat, food companies require rapid and efficient methods to verify the composition of soybeans received for processing. Traditional laboratory-based techniques, such as Gas Chromatography with Flame Ionization Detection (GC-FID), are time-consuming, costly, and require skilled personnel.

Near-infrared (NIR) spectroscopy offers a fast, non-destructive alternative for measuring key soybean parameters. This study demonstrates the effectiveness of ProxiScout™ in analyzing soybean samples to determine their oleic and linoleic acid content, providing a valuable tool for on-site quality assessment.

2. Equipment

The ProxiScout™ handheld NIR scanner was used to collect spectral data from soybean samples. The device enables real-time quality control and screening with minimal training, utilizing diffuse reflectance spectroscopy to capture spectral fingerprints.

- Setup: Diffuse reflection.
- Spectral Range: 1350–2550 nm.

3. Samples and Measurement Conditions

3.1 Sample Collection

- Total Samples: 88 soybean samples collected from four different suppliers.
- Sample Types:
  - Conventional soybeans.
  - High-oleic soybeans.
- Environmental Testing: Two whole soybean samples were stored at -20 °C, 4 °C, and 20 °C to assess model performance under extreme temperature variations.

3.2 Measurement Conditions

- Scan Time: 5 seconds per sample.
- Resolution: 16 nm at λ = 1,550 nm.
- Spot Size: 10 mm^2.
- Temperature: Room temperature.
- Averaging: The ground sample was measured 6 times, while whole soybeans were measured 12 times, with results averaged for analysis.

4. Procedure

4.1 Reference Methods

Gas Chromatography (FID) was used to analyze the fatty acid profile from the ether-extracted fat. Results are expressed in grams of fatty acid per 100 g of sample. The reference laboratory values were used to calibrate and validate the NIR-based predictive models.

Table 1: Constituent description.

Parameter	N	Mean	SD	Min	Max
Linoleic	88	6.02	4.89	0.62	14.8
Oleic	88	11.48	5.88	3.17	20.74

4.2 Calibration Model Development

Partial Least Squares (PLS) regression models were developed to establish a linear relationship between spectral data and laboratory-measured oleic and linoleic acid content. The models were optimized using:

- Cross-validation techniques to enhance predictive accuracy.
- Generalized sample calibration, ensuring robustness against unit-to-unit variability and environmental effects such as temperature changes.

4.3 Data Analysis

The PLS model was evaluated using cross-validation, which involved splitting the data into calibration and validation sets, training the model, and testing its performance. Statistical parameters included:

- R^2 (Coefficient of Determination): Measures how well-predicted values match actual values (closer to 1 is better).
- RMSE (Root Mean Square Error): Represents prediction error (lower is better).
- Bias: Measures deviation from actual values (closer to 0 is ideal).

5. Result

5.1 Model Performance Metrics

Results from the cross-validation are shown in Figure 1. In order to quantify the accuracy of the model, the following statistical characteristics are summarized in:

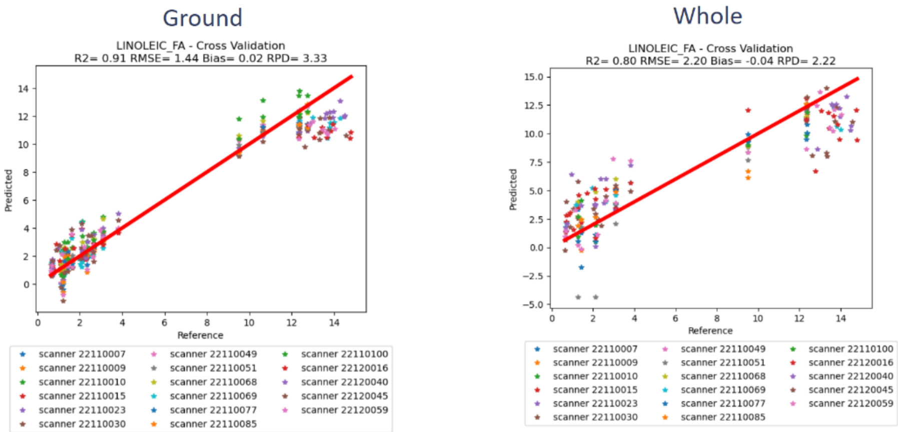

Figure 1: The relation between the reference data (chemical analysis) and the predicted results from our model. Each dot represents a test sample where X-coordinate is the reference value, and the y-coordinate is the model prediction. The red line represents the ideal model and R^2 (ideal value is 1) shows how far the model deviates from the ideal one. a) For linoleic acid and b) for oleic acid.

The findings presented in this study suggest that the Scanner provides excellent results in predicting ground samples. Moreover, whole soybeans can be analyzed for a quick analysis providing a screening tool without sample preprocessing (Table 2).

Table 2: Performance of the calibration model and the cross-validation statistic.

Parameter	Type	SEC	R^2CV	SECV	SD/SECV
Linoleic	*Whole*	1.89	0.80	2.20	2.69
-	*Ground*	1.36	0.91	1.44	3.45
Oleic	*Whole*	2.46	0.80	2.86	3.02
-	*Ground*	1.64	0.90	1.84	4.04

Table 3: Performance of the calibration model and the cross-validation statistic.

ID	Temperature	Linoleic	Oleic
Sample A	*Freezer*	*4.1*	*13.3*
	Fridge	*3.3*	*14.3*
	Room temperature	*3.9*	*13.6*
Sample B	*Freezer*	*4.6*	*12.8*
	Fridge	*3.7*	*14.1*
	RT	*5.5*	*11.9*
Standard deviation		*0.63*	*0.77*
Model's CV RMSE		*2.2*	*2.86*

5.2 Key Observations

- The ProxiScout™ scanner successfully differentiated between high-oleic and conventional soybeans.
- Whole soybeans can be analyzed for rapid screening, while ground soybeans provide enhanced accuracy.
- The temperature variation study confirmed model robustness, with minimal deviations across different temperature conditions.

6. Conclusion

6.1 Comparison to Standard Methods

- ProxiScout™ results closely matched GC-FID measurements, validating its suitability for on-site screening.
- Unlike laboratory methods, ProxiScout™ provides instant results, eliminating sample transport and preparation delays.

The ProxiScout™ handheld NIR scanner has demonstrated excellent performance in assessing soybean quality, distinguishing high-oleic from conventional soybeans with high accuracy. Its ability to analyze both whole and ground samples makes it a versatile tool for soybean processors, quality control laboratories, and food manufacturers. The integration of real-time data collection and cloud storage ensures seamless monitoring across the supply chain.

7. References

[1] Roberts, C. A., Ren, C., Beuselinck, P. R., Benedict, H. R., & Bilyeu, K. D. (2006). Fatty acid profiling of soybean cotyledons by near-infrared spectroscopy. Journal of Applied Spectroscopy, 60, 1328–1333. USDA Data on Soybean Production and Fatty Acid Profiles

[2] Shenk, J. S., Workman, J. J., & Westerhaus, M. O. (2001). Application of NIR spectroscopy to agricultural products. Practical Spectroscopy Series, 27, 419–474. Gas Chromatography for Fatty Acid Analysis

[3] Murray, I., & Williams, P. C. (1994). Chemical principles of near-infrared technology. In P. C. Williams & K. Norris (Eds.), Near-Infrared Technology in the Agricultural and Food Industries (pp. 17–34). NIR Spectroscopy in Oilseed Quality Control

[4] Kessler, H.-G.: Lebensmittel-und Bioverfahrenstechnik, Molkereitechnologie, Verlag A. Kessler, Freising, 4. Auflage 1996.