10th Brazilian Conference on Natural Products
XXXVI RESEM
4-7 November 2025, Belo Horizonte, MG, Brazil

Section:

NIR SPECTROSCOPY FOR EFFICIENT SCREENING OF BIOACTIVE COMPOUNDS IN SORGHUM

Maria Lúcia Ferreira Simeone[1*], Valéria Aparecida Vieira Queiroz[1], Rafael de Araújo Miguel[1], Thaís Fernanda Silva[2], Emilly Rodrigues De Souza Santos[2], Cícero Beserra de Menezes[1], Maria Marta Pastina[1]
marialucia.simeone@embrapa.br

1-EmbrapMilho e Sorgo, Rod MG 424, Sete Lagoas, MG, 35701-970, Brazil.
3- Universidade Federal de São João Del Rei, Campus Sete Lagoas, Minas Gerais, Brazil.

In recent years, there has been a growing interest in using sorghum for human consumption, mainly due to the demand for healthier, gluten-free foods with greater nutritional value. In addition, sorghum is a source of bioactive compounds with antioxidants, immunomodulatory, anti-inflammatory, and antimicrobial properties. The chemical characteristics of bioactive compounds become critical for human nutrition purposes, which influence their bioavailability and differ among sorghum genotypes. The reported high phenolic levels in sorghum have led to interest from sorghum breeding programs in developing and identifying germplasms with high phenolic levels, which requires screening many samples to find those with the highest levels. Since wet chemistry screening methods are slow, expensive, and destructive, the use of near-infrared (NIR) spectroscopy calibration models could be an alternative. The objective of this study was to develop NIR models for total phenols, condensed tannins, antioxidant activity, and total anthocyanin levels in a diverse set of ground grains of the 240 sorghum genotypes, and to assess the predictive value of NIR models to estimate these compounds in sorghum. A calibration model was developed using (NIRFlex 500, Buchi) (1,000 to 2,500 nm) and a chemometrics approach. Each compound estimated using NIR models was validated using an independent validation set. Calibration models correlations for total phenols, condensed tannins, antioxidant activity, and total anthocyanins were R^2 = 0.91, 0.84, 0.84, and 0.82, respectively. Correlations between NIR-predicted values and reference values in the validation set were significant for total phenols (R^2 = 0.90), condensed tannins (R^2 = 0.83), antioxidant activity (R^2 = 0.82), and total anthocyanins (R^2 = 0.80). They indicated that sufficient variation for these compounds existed within sorghum and that NIR calibration models could be used to rapidly and non-destructively predict total phenols, condensed tannins, antioxidant activity, and total anthocyanins concentrations in ground grain sorghum.

Acknowledgments
We are grateful for the funding provided by CAPES, CNPq **Processo:** 423300/2021-0, FAPEMIG, and Embrapa.

Keywords: *Sorghum bicolor, functional foods, chemometrics,near-infrared, chemometrics*