

Spectroscopy methods for discrimination of specialty coffee quality: NIR vs. FTIR

Franca Adriana¹ (adriana@demec.ufmg.br), Belchior Veronica², Botelho Bruno³

S8-PO-02



¹PPGCA, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil; ²DQ, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil

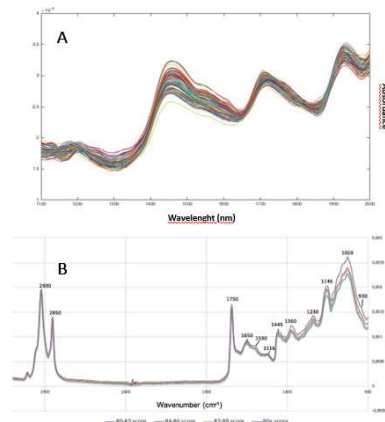


Figure 1: (A) NIR (900-2300 nm) and (B) FTIR Full spectra (3000–900 cm⁻¹) of roasted coffee in original scale.

Results/Discussion. PLS models were built, and although both NIR and FTIR were able to provide good predictions, the FTIR results were more accurate, providing consistent models for predicting cup quality based on the SCA sensory analysis, with low values of RMSEC and RMSEP (0.23 both for FTIR and 0.50 both for NIRS). Also, the FTIR models showed slightly higher values of calibration ($R_c - 0.99$) and validation ($R_v - 0.97$) coefficients in comparison to NIR results ($R_c - 0.98$ and $R_v - 0.96$).

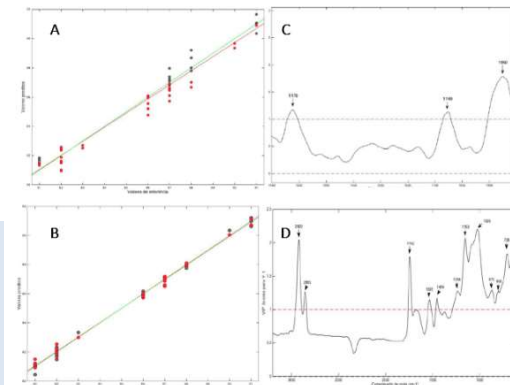


Figure 2: Experimental versus predicted values by the PLS models of the data submitted to The OSC, SNV, and mean center: (A) NIR, (B) FTIR, and their respective VIP Scores (C) NIR, (D) FTIR.

Introduction. The Specialty Coffee Association (SCA) sensory analysis protocol is the official methodology employed to classify specialty coffees. However, because sensory analysis is sensitive to the taster's training, cognitive psychology and physiology, among other parameters, the feasibility of instrumental approaches has been recently studied for complementing such analyzes. Spectroscopy methods, mainly near infrared (NIR) and mid infrared (FTIR – Fourier Transform Infrared), have been extensively employed for food quality authentication. In view of the aforementioned, in the present study we compared NIR and FTIR to distinguish different qualities and sensory characteristics of specialty coffee samples.

Materials/Methods. Samples of specialty coffee were provided by Federação dos Cafeicultores do Cerrado Mineiro and Fazenda Barinas (n=28), roasted in IKAWA coffee roaster (in duplicate, n=56) and submitted to NIR analysis (two fractions of each sample were analyzed, providing a total of 112 spectra in the range of 900 to 2300 nm). The beverage was prepared in accordance with the SCA protocol, tasted by a group of Q-graders and submitted to FTIR analysis. Two fractions were withdrawn from each sample and analyzed in duplicate, totaling 224 spectra in the range of 4000 to 600 cm⁻¹ (56 beverages x 2 aliquots x 2 analysis).

Conclusion/Perspectives. The results confirmed the feasibility of both techniques for predicting specialty coffee quality. In general, FTIR results were more accurate, but either technique could be implemented by the coffee industry. The prediction of coffee roasting profile and its quality is of significant importance for the validation of specialty coffee quality.

References. [1] Belchior V, Botelho BG, Oliveira LS, Franca AS (2019). *Food Chem* 273:178–185. [2] Craig AP, Botelho BG, Oliveira LS, Franca AS (2018). *Food Chem* 245:1052–1061. [3] Gloess AN, Vietri A, Wieland F, Smrke S, Scön bächler B, López JAS, Petrozzi S, Bongers S, Kozirowski B, Yeretian C (2014). *Mass Spectrom* 365–366:324–337.