

Title: APPLICATION OF FOURIER TRANSFORM MID-INFRARED SPECTROSCOPY FOR IDENTIFICATION OF *Aspergillus* SPECIES ISOLATED FROM COFFEE BEANS

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Abstract:

In mycology, one of the challenges is to differentiate similar species. Morphology-based methods are often limited, thereby increasing the demand for new field explorations to obtain better and more reliable results. Fourier Transform Infrared (FT-IR) spectroscopy is proposed as an alternative method for the classification of highly related fungi such as *Aspergillus ochraceus* and *Aspergillus westerdijkiae* or *Aspergillus carbonarius* and *Aspergillus niger*. However, methodologies for sample preparation are time consuming and laborious. In this study, a traditional method for sample preparation was adapted by reducing the time and maintaining the quality of analysis, in addition, a chemometric model was developed. The fungi were grown in Sabouraud medium for 4 days, the mycelium was blended with KBr and analyzed by Fourier Transform Mid-Infrared Transmittance (FT-MIR) spectroscopy. Partial Least Squares regression was applied to the species comparison models and a prediction test was used to evaluate the models. The Coefficient of Determination for Calibration and Root Mean Square Error of Calibration were 0.94 and 0.23, respectively. In the external validation the model correctly classified 88.88% of the samples, with a Prediction Root Mean Square Error of 0.35; only one *A. westerdijkiae* was not correctly classified. The chemometric model on the basis of FT-MIR spectra transmittance developed was able to correctly distinguish between highly related species such as *A. niger* and *A. carbonarius*. However, due to the chemical similarity between *A. ochraceus* and *A. westerdijkiae*, the differentiation of these two species was not possible in all cases. The difficulty in differentiating *A. ochraceus* and *A. westerdijkiae* is also observed when morphological, physiological and molecular biological analyses are performed. The adaptation of traditional method of sample preparation proved to be very fast, being completed in 4 days, and easy to apply, with few processing steps.

Keywords: *Aspergillus*; coffee beans; spectroscopy; identification.

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