

Rapid determination of potential aflatoxigenic fungi contamination on peanut kernels during storage by data fusion of HS-GC-IMS and fluorescence spectroscopy

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Abstract

This study described the rapid determination of potential aflatoxigenic fungi contamination on peanut kernels based on headspace-gas chromatography-ion mobility spectrometry (HS-GC-IMS) coupled to fluorescence spectroscopy. Data-level and feature-level fusion strategies were introduced to integrate HS-GC-IMS and fluorescence spectra, aiming at improving the performances of identification and prediction models. The application of feature-level data fusion using first 10 PCs coupled with orthogonal partial least squares discriminant analysis (OPLS-DA) offered more accurate characterization (96.7 %) for aflatoxigenic and non-aflatoxigenic fungal infection on peanut samples. Regression models were established for predicting colony counts of peanuts infected with aflatoxigenic fungi based on independent and fused signals by partial least squares regression (PLSR). Feature-level data fusion using first 10 PCs achieved the best performances in colony counts predictions for *A. flavus* ($R^2 = 0.950$) and *A. parasiticus* ($R^2 = 0.971$). These results demonstrated that the combination of HS-GC-IMS and fluorescence spectra might offer the feasibility for early detection of potential aflatoxigenic risk in peanuts.