Abstract

In the present study, the capibility of near-infrared spectroscopy and hyperspectral imaging technology have been investigated to detect and evaluate some cocoa bean quality parameters. In the first part of the research, the amount of polyphenolic compounds and cocoa bean fermentation index were evaluated. For this purpose, an infrared spectrometer in the range of 400 to 2500 nm was used and in order to provide a suitable model for predicting polyphenolic materials, a number of different pretreatments were evaluated. Among these models, the model with the pretreated spectrum of the second derivative of Savitzky-Golay, has the highest coefficient of determination 0.9 and error 1.9 for calibration data and coefficient of determination 0.81 and error 1.94 for data test introduced. In predicting the fermentation index, the PLS model presented with the second derivative spectral pretreatment had the highest coefficients of determination 0.82, 0.42 and the lowest error rates of 0.06 and 0.17 for calibration and test data. In the second part of the study, near-infrared spectroscopy was used as a non-destructive method to detect aflatoxin-contaminated cocoa beans. Cocoa beans were artificially contaminated with two concentrations of toxin (20 ppb and 500ppb) and uninfected beans (0 ppb) were superficially purified with ethanol. Both groups of infected and healthy grains were evaluated with a spectrometer in the range of 400 to 2500 nm. The partial least squares discriminant analysis model (PLS_DA) was used to classify infected and non-contaminated grains, and before analyzing the spectral data, these spectra were pretreated with the first and second order derivatives of Savitzky-Golay. The calibration results showed that the lowest calibration error was in the case that the second-order derivative was used as pretreatment and these values for calibration, cross-validation and test data were 0.02 ، 0.02, respectively. In the final part of the research, using spectral imaging technology, four groups of foreign materials (wood and paper, plastic, stone and plant organs) that are common in the cocoa bean processing industry were identified and classified. For this purpose, spectral image data of 250 samples of foreign materials and cocoa beans, using principal component analysis and three classification models including: Support Vector Machines (SVM), K Nearest Neighborhood (KNN) and Linear Discrimination Analysis (LDA) were evaluated. The optimal wavelengths obtained from the second derivative of the spectrum as well as the first three components (PCA) were introduced as input into the class models and the performance of these models was compared with each other. The results showed that the SVM model with the input of raw spectrum without preprocessing, was able to correctly classify samples of foreign materials and cocoa beans with the highest accuracy (89.10%). The accuracy of this model when it used the optimal wavelengths as its input was equal to 86.9% for the calibration data and 81.28% for the test data. The results of this experiment also showed that in our data sets, if the optimal wavelengths are used as input to the classification model, the classification efficiency can be more stable.

Keywords : Near infrared spectroscopy, Hyperspectral imaging, Aflatoxin B1, Foreign matter, Cocoa beans