微量有机磷农药残留近红外光谱快速检测方法 Determination of Organophosphorus Pesticide Residue by Using Near-infrared Spectroscopy

陈菁菁 李永玉 王伟 彭彦昆 吴建虎 单佳佳

中国农业大学

关键词：　　有机磷农药 近红外光谱 偏最小二乘回归法 快速检测

摘　要：　　以滤纸作为农药载体，在波数4 000～10 000 cm-1 范围内获取其近红外光谱曲线。分别采取偏最小二乘回归法和最佳波段差值回归法建立农药质量比的预测模型。偏最小二乘回归法在经过多元散射校正和变量标准化预处理后得到的预测结果较好，预测相关系数为0.954，通过最佳波段差值回归法得到的预测相关系数为0.904。两种建模方法都得到了较好的预测结果。 Near-infrared (NIR) spectroscopy was used to measure trace chemicals, which could be useful for detection of pesticide residue in vegetable. Filter paper was used as the substrate. Pesticide solution was prepared by dissolving the commercial pesticide into distilled water at different concentrations. Samples were prepared by pipetting the solution onto the filter paper and then evaporated by vacuum drying oven. Then the spectra of samples were acquired in the region of 4000 cm-1 to 10000 cm-1 by NIR spectrometer. Partial least squares regression (PLSR) method and optimal band difference regression (OBDR) were used to establish prediction models respectively. Prediction results indicated that the PLSR models were able to predict the concentration of chlorpyrifos with 0.954 as the correlation coefficient of validation set, the OBDR models gave the best performance with 0.904 as the correlation coefficient of validation set. It could be concluded that NIR determination of pesticide was a low cost, environment friendly and potential method compare to the traditional methods.

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