

醋糟有机基质含水率的可见/近红外光谱检测 Detection of Moisture Content in Vinegar Residue Substrate Using Visible-near-infrared Spectroscopy

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关键词: 醋糟 有机基质 含水率 偏最小二乘法 近红外光谱

摘要: 以醋糟有机基质为研究对象, 采用便携式可见/近红外光谱仪采集了不同含水率基质样品(69个)的漫反射光谱, 通过选择不同的光谱预处理方法并确定其主成分数, 建立了基于偏最小二乘法(PLS)的醋糟基质含水率定量分析模型。结果表明, 以滑动平均滤波(MAF)和一阶微分(FD)相结合作为原始光谱的预处理方法所建立的模型(主成分数为5)对基质含水率的检测效果较好, 其校正模型和预测模型决定系数分别为0.9930和0.9901, 校正均方根误差(RMSEC)和预测均方根误差(RMSEP)分别为0.0676和0.0715。因此, 可见/近红外光谱技术可以作为醋糟有机基质含水率快速检测的一种可靠方法。 In order to develop a method for rapid detection of moisture content in vinegar residue substrate, the spectral data of 69 representative samples were collected by using visible-near-infrared spectroradiometer, and the oven-drying method was applied to obtain the data of these samples moisture content. Partial least squares regression (PLS) method was selected to perform the calibration models for predicting the moisture content. For determining the number of principal component factors in the PLS model and the method of spectra preprocessing, the model with the lowest prediction residual error sum of square based on cross-validation for the calibration samples set was chosen. The determination coefficient between the predicted and the reference results for the prediction samples set, along with the root mean squared error of prediction (RMSEP), was used as evaluation parameters for the models. The results indicate that the forecast result of spectral data is optimal through the spectra preprocessing method of moving average filter (MAF) and first derivative (FD), with 5 principal component factors. The determination coefficients of the calibration and prediction models are 0.9930 and 0.9901, with root mean squared error of calibration (RMSEC) and prediction (RMSEP) of 0.0676 and 0.0715, respectively. Therefore, visible-near-infrared spectroscopy with PLS method can be used successfully to determine the moisture content of vinegar residue substrates.

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