花椒挥发油含量的近红外光谱无损检测

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关键词： 花椒 挥发油含量 近红外光谱分析 无损检测

摘 要： 应用近红外漫反射光谱技术，采用偏最小二乘法，针对118份完整花椒颗粒定标样品集，研究了扫描分辨率为4、8、16 cm-1 ，扫描次数为32、64、128的9种扫描参数组合情况下的挥发油含量近红外光谱预测模型。扫描分辨率为16 cm-1 、扫描次数为128时，建立的预测模型最优。在最优参数组合情况下，定标集样品的内部验证决定系数R2为0.907，交互验证误差均方根为0.509，用20份样品作为预测集进行外部验证，外部验证决定系数 R2为0.973，预测误差均方根为0.272，相对分析误差为6.28。结果表明，近红外光谱分析技术可以快速、无损地检测花椒颗粒中挥发油的含量。The method of near infrared reflectance spectroscopy for predicting volatile oil content in intact Zanthoxylum bungeagum Maxim was developed. Adopting partial least squares (PLS) regression, the prediction models were built by the 118 samples in 9 kinds acquisition parameters combination with the resolution (4, 8 and 16cm-1) and the sample scans (32, 64 and 128). Results demonstrated that the model obtained at resolution of 16 cm-1and sample scans of 128 was better than the others, and the determination coefficient and RMSECV of cross validation were 0.907 and 0.509, respectively. Applying the model to the test set with 20 samples, the determination coefficient, RMSEP and RPD of test set validation were 0.973, 0.272 and 6.28, respectively. The experimental results show that NIRS can be used as a method to detect intact Zanthoxylum bungeagum Maxim volatile oil content rapidly and nondestructively.

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