

黄酒总糖含量的中红外光谱定量检测 Determination of Total Sugar Content in Chinese Rice Wine by Mid-infrared Spectroscopy

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摘要: 利用中红外光谱技术对黄酒中的总糖含量进行了快速检测。实验以3个厂家的共30个样品为研究对象, 在1000~1500cm<sup>-1</sup> 和2500~3000cm<sup>-1</sup> 波段范围内建立了多元线性回归、主成分回归以及偏最小二乘回归模型, 并比较了微分的光谱预处理方法对模型精度的影响。二阶微分光谱建立的偏最小二乘模型的精度最佳, 交互验证的相关系数为0.984, RMSECV为0.765g/L, RPD为5.75, 表明中红外光谱技术可以用于黄酒中总糖含量的快速检测。Mid-infrared spectroscopy combined with chemometrics was used to determine total sugar content in Chinese rice wine. A total of 30 samples were collected. Calibration models were developed in the range of 1000cm<sup>-1</sup> to 1500cm<sup>-1</sup> and 2500 cm<sup>-1</sup> to 3000cm<sup>-1</sup> to exclude the influence of water absorption. Stepwise multiple regression (SMLR), principal component regression (PCR) and partial least squares regression (PLSR) were used to develop the models in TQ analyst software. And derivative pretreatment method was used to test the impact of accuracy of the models established. The best model was obtained by PLSR with second-order derivative pretreatment. The correlation coefficient of cross validation (rcv) was 0.984, RMSECV to 0.765g/L, RPD to 5.75. The result indicates that mid-infrared spectroscopy (MIR), combined with chemometric methods, can be used as a fast, simple and exact method to measure total sugar content in Chinese rice wine.

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