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近红外光谱快速检测食用油必需脂肪酸

Rapid determination of essential fatty acids in edible oils based on near infrared spectroscopy

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中文关键词:近红外光谱,模型,优化,α-亚麻酸和亚油酸,食用油,检测

英文关键词:near infrared spectroscopy models optimization α-linolenic acid and linolenic acid edible oils determination

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中文摘要:

为了建立食用油必需脂肪酸快速检测的方法,该研究提出了基于近红外光谱技术检测食用油中α-亚麻酸和亚油酸含量的快速测定方法。对光谱信息分别采用偏最小二乘回归方法(PLS)和最小二乘支持向量机(LS-SVM)建立模型。比较了多种光谱预处理方法对模型预测能力的影响。结果表明对于亚油酸含量的预测,采用Savitzky-Golay平滑法结合多元散射校正(MSC)的光谱预处理所建立的LS-SVM模型最优。预测集的决定系数(R2)、预测均方根误差(RMSEP)和剩余预测偏差(RPD)分别达到了0.9 89,0.0161和9.4783。对于α-亚麻酸含量的预测,采用Savitzky-Golay平滑法结合标准正态变换(SNV)的光谱预处理所建立的LS-SVM模型最优。α-亚麻酸含量预测结果的R 2、RMSEP和RPD为0.972,0.0036和6.0561,据此表明,应用近红外光谱技术能够检测食用油中α-亚麻酸和亚油酸的含量,为快速检测食用油的必需脂肪酸提供了参考。

英文摘要

In order to find out a fast quantitative determination method for the essential fatty acids in edible oils, near infrared spectroscopy was applied in determination of the contents of α -linolenic acid and linoleic acid. The chemometrics models between near infrared spectra and the contents of α -linolenic acid and linoleic acid were established by partial least squares regression (PLS) and least-squares support vector machine (LS-SVM). Several common used spectral pretreatment methods were used to establish different PLS and LS-SVM models. For linoleic acid prediction, best predictive performance was obtained using LS-SVM model and spectral pretreatment of Savitzky-Golay smoothing and multiplicative scatter correction (MSC). Coefficient of determination (Rp2), root mean square error for prediction (RMSEP) and residual predictive deviation (RPD) were 0.0161, 0.989 and 9.4783, respectively. For α -linolenic acid prediction, best predictive performance was obtained using LS-SVM model and the spectral pretreatment of Savitzky-Golay smoothing and standard normal variation (SNV). Rp2, RMSEP and RPD were 0.0036, 0.972 and 6.0561, respectively. The results indicate that it is feasible to use near infrared spectroscopy for fast determination of α -linolenic acid and linoleic acid contents in edible oils.

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