

## 近红外光谱分析法测定菜籽油中芥酸的含量

### Determination of the erucic acid content in rapeseed oil by near-infrared spectroscopy

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作者	单位
陈蛋	(1979-), 男, 研究方向是近红外技术在食品的无损检测应用研究。镇江江苏大学生物与环境工程学院, 212013
陈斌	(1960-), 男, 博士, 教授, 博士生导师, 主要从事近红外光谱技术在食品和农产品应用的研究。镇江江苏大学生物与环境工程学院, 212013。Email:ncp@ujs.edu.cn
陆道礼	江苏大学生物与环境工程学院, 镇江 212013
钟旭美	陕西师范大学食品工程系, 西安 710062

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中文摘要:

采用多通道PDA型近红外光谱仪,应用偏最小二乘法建立了菜籽油中芥酸含量与近红外透射光谱的校正模型,讨论多项式求导及平滑的窗口宽度和相关系数法筛选有效波长对校正模型的影响,并对10个预测集样品利用预测相关系数 $R_p$ 和预测均方根误差RMSEP指标进行了预测精度分析,结果发现:在使用全谱数据进行偏最小二乘回归建模时,一阶7点求导及平滑的预处理方法结果最佳,此时建模效果为: $R_p=0.739$ , $RMSEP=1.659$ ;在此基础上通过相关系数法筛选波长后的建模效果为: $R_p=0.958$ , $RMSEP=0.963$ 。后者 $R_p$ 提高29%, $RMSEP$ 减少42%。由此可得出多项式求导及平滑法和相关系数法相结合对校正模型稳健性,预测精度都有较大提高的结论。研究证明:多通道近红外光谱仪快速测定菜籽油中芥酸含量的方法是可行的。

英文摘要:

In this paper, the erucic acid content of rapeseed oil and the correction model of near-infrared transmission spectrum were established based on partial least square(PLS) method by using multichannel PDA near-infrared spectroscopy instrument. The influences of window size of polynomial derivation and smoothing and wavelength selected by correlation coefficient on the correction model were discussed. The predicted precisions of ten samples were analyzed by the index of predicted relative coefficient( $R_p$ ) and root-mean-square error(RMSEP). The result showed that the first derivation with seven points and smooth pretreatment is the best while adopting PLS modeling on the whole spectra, and the results of  $R_p$  and RMSEP are 0.379 and 1.659, respectively. When selecting wavelength by relative coefficient,  $R_p$  and RMSEP are 0.958 and 0.963, respectively. Compared with the results of the two methods, the latter  $R_p$  improves by 29% and RMSEP reduces by 42%. Therefore, the conclusions can be drawn that combining polynomial derivation and smooth pretreatment with correlation coefficients will improve the steadiness and predicted precisions of correction model. It shows that it is feasible to quickly determine the erucic acid content in rapeseed oil by multichannel near-infrared spectroscopy.

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