论文

二维相关近红外谱结合NPLS-DA判别掺杂牛奶的研究

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摘要：

将二维相关近红外谱与多维偏最小二乘判别分析方法结合起来,建立了掺杂牛奶与纯牛奶的判别模型.分别配置掺杂尿素牛奶(1~20 g/L)和掺杂三聚氰胺牛奶(0.01~3 g/L)样品各40个,采集纯牛奶及掺杂牛奶样品的近红外光谱.在量化二维相关近红外同步谱的基础上,采用多维偏最小二乘判别分析法分别建立了掺杂尿素、掺杂三聚氰胺及两种掺杂牛奶与纯牛奶的判别模型对未知样品进行判别,其判别正确率分别为95%、90%和92.5%,并与偏最小二乘判别和隐变量正交投影判别建模方法进行了比较.结果表明:多维偏最小二乘判别分析法具有更强的预测能力可推广到其它食品的掺杂检测中.

关键词： 二维相关近红外谱　多维偏最小二乘判别分析　掺杂牛奶　尿素　三聚氰胺

Discrimination of Adulterated Milk Using NPLS-DA Combined with Two-dimensional Correlation Near-infrared Spectroscopy

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Abstract:

In order to develop a rapid, cost-effective and high-throughput analysis method for detecting adulterants in milk, adulterated milk discriminant models are established by combing two-dimensional (2D) correlation near-infrared spectroscopy with multi-way partial least squares-discriminant analysis (NPLS-DA). 40 adulterated milk samples with melamine (0.01~3 g/L) and 40 adulterated milk samples with urea (1~20 g/L)are prepared respectively, then the absorption spectra of all samples are measured. Based on quantization of 2D correlation spectrum, the NPLS-DA models of urea-tainted milk, melamine-tainted milk and two types adulterated milk are constructed. The recognition rates of unknown samples are 95%, 90%, and 92.5% by calibration models individually. At the same time, PLS-DA and OPLS-DA models are established. The results show that NPLS-DA model has better predictive ability than PLS-DA model and OPLS-DA model, and this method can also be applied to other food safety detection areas.

Keywords: Two-dimensional correlation near-infrared spectroscopy　NPLS-DA　Adulterated milk　Urea　Melamine

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