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现代应用光学

红外光谱结合核隐变量正交投影法判别掺杂牛奶

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摘要: 为了快速、准确地检测掺杂牛奶, 采用基于核隐变量正交投影(K-OPLS)法分析了掺杂牛奶的光谱。选用高斯函数作为核函数, 内部交叉验证均方根(RMSECV)最小值作为评价指标, 优选了核函数中的核宽度 σ 以及Y正交成分数。配置含四环素牛奶(0.01~0.3 gL⁻¹)、三聚氰胺牛奶(0.01~0.3 gL⁻¹)和葡萄糖牛奶(0.01~0.3 gL⁻¹)各36个, 采集纯牛奶及掺杂牛奶样品的红外光谱, 采用K-OPLS建立各掺杂牛奶与纯牛奶的判别模型。利用这些模型对未知样品进行判别, 结果显示对掺杂四环素、三聚氰胺、葡萄糖牛奶的判别正确率分别为100%、100%、95.8%。建立了同时判别3种掺杂牛奶与纯牛奶的K-OPLS模型, 该模型对未知样品的判别正确率为93.1%; 同时, 与偏最小二乘判别PLS-DA方法的预测结果进行了比较, 结果表明: K-OPLS建模方法对于复杂的牛奶体系具有较好的预测能力。

关键词: 红外光谱 核隐变量正交投影 掺杂牛奶 四环素 三聚氰胺 葡萄糖

Discrimination of Adulterated Milk Based on Infrared Spectroscopy and K-OPLS

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Abstract: To detect adulterated milk rapidly and accurately, the discrimination models for adulterated milk were established based on the method of Kernel Orthogonal Projection to Latent Structure (K-OPLS). By using the Gaussian radial basis function as the kernel function and the minimum value of Root Mean Square Errors of Cross-validation (RMSECV) as an evaluation index, the width of the Gaussian kernel, the minimum value of the RMSECV, and the number of Y-orthogonal components (scalar) were selected in a optimization. 36 samples with different concentrations of tetracycline (0.01-0.3 gL⁻¹), melamine (0.01-0.3 gL⁻¹) and glucose (0.01-0.3 gL⁻¹) in milk were prepared, respectively. Then the infrared absorption spectra of all samples were measured. K-OPLS models for tetracycline-tainted milk, melamine-tainted milk and glucose-tainted milk were constructed. The results show that its classification accuracy for tetracycline-tainted milk, melamine-tainted milk and glucose-tainted milk are 100%, 100%, 95.8%, respectively. The K-OPLS model was used to classify the above three kinds of adulterated milk and pure milk and its classification accuracy for unknown samples is 93.1%. Compared with Partial Least Square Discriminant Analysis (PLS-DA), K-OPLS methods show higher accuracy. The results indicate that the K-OPLS model has good prediction ability for complex milk systems.

Keywords: infrared spectroscopy Kernel Orthogonal Projection to Latent Structure (K-OPLS) Adulterated milk tetracycline Melamine Glucose

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