

研究论文

基于多模型共识的偏最小二乘法用于近红外光谱定量分析

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摘要 建立了多模型共识偏最小二乘(cPLS)建模方法, 并应用于烟草样品近红外(NIR)光谱与常规成分氯含量之间的建模研究, 探讨了建模参数对预测结果的影响. 结果表明, cPLS方法与传统的偏最小二乘算法(PLS)相比, 所建模型更稳定可靠, 预测结果也可得到了明显改善.

关键词 [多模型共识](#) [偏最小二乘法](#) [近红外光谱](#) [烟草样品](#) [定量分析](#)

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Partial Least Squares Regression Method Based on Consensus Modeling for Quantitative Analysis of Near-Infrared Spectra

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Abstract Consensus modeling averages the results of multiple independent models to obtain a single prediction, which avoids the instability of a single model. Based on the philosophy of consensus modeling, a consensus partial least squares regression(cPLS) method was proposed and applied to building the quantitative model of NIR spectra of tobacco samples. Through an investigation of the parameters involved in the modeling, a satisfied model was achieved for predicting the content of chlorine in tobacco samples. With repeated independent runs, cPLS model was found to be more robust and credible than PLS model. Furthermore, compared with PLS method, cPLS model gives more stable and accurate prediction results.

Key words [Consensus modeling](#) [Partial least squares](#) [Near-infrared spectroscopy](#) [Tobacco sample](#) [Quantitative analysis](#)

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