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Adaptive noise model based iteratively reweighted penalized least squares for fluorescence background subtraction from Raman spectra

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Abstract

The spectral analysis depends heavily on unwanted signals, such as the fluorescent background from the samples or other interfering components. A number of mathematical algorithms have been proposed to remove the background of Raman spectra. However, these methods require the selection of appropriate parameters to correct the of Raman spectra baseline. In this paper, we propose a method of adaptive noise model based on iteratively reweighted penalized least squares (ANM-IRPLS) for Raman spectrum baseline correction. The algorithm was applied to various artificial spectra containing real forms of baselines and characteristic Raman peaks and then to the spectra of real drug samples with fluorescence obtained on a device equipped with a 532-nm laser with a resolution of 15 cm−1. The modeling results showed that the proposed ANM-IRPLS baseline correction method allows for better results in background removal than the airPLS. For real Raman spectra processed by the ANM-IRPLS method, it is shown that the algorithm handles a complex background well, while maintaining the characteristic Raman signal features, such as a wide water peak for aqueous solutions.

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Keywords

background subtraction, fluorescence background, iteratively reweighted penalized least squares, mathematical processing of spectra, Raman spectroscopy

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