Identification of Location of Peaks in the Pure Spectrum from Multi Component Data

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Application of multivariate calibration is very important to measure or predict the amount of quantitative information in areas, such as chemistry, medicine, pharmacy, agriculture, spectroscopy, biomedical engineering, working on materials consisted of many components. In such applied areas, for saving of cost and time, and avoiding complication, it is necessary to use easier method like absorption spectra transmitted by light rather than by direct method like use of chemicals or blood-drawing. A primary concern about easier method is how to extract qualitative information like location of peaks of pure spectrum of a target component from a mixture of multicomponents. It is necessary to provide the accurate estimation of the amount of quantitative information. But, it is not easy to identify the location of peaks in the pure spectrum of a component due to the interferent components.

In this situation, a method identifying the location of peaks in the pure spectrum of the component of interest was developed. This method used the regression vector changes as a function of the overlap between the pure spectra of the components in the samples with classical calibration (CLS) model assuming no noise(Seasholtz, and Kowalski, 1990). So, it is rather theoretical, and not practical to use.

With multicomponent data, this study considers the method to identify the location of peaks in the pure spectrum of a target component in the samples with spectral noise. This method is validated with various simulated data sets. Simulated data sets are generated according to the extent of overlap of peaks between target component and interferent component, the ratio of intensities of two components.

The results of the study contribute to the valid qualitative analysis and the accurate quantitative analysis by mathematical, and statistical method, and to the accurate analysis of clinical and chemical component in medicine, soil or air component in environment area, and oil component in oil refining industry.

REFERENCE

1. M. B. Seasholtz and B. R. Kowalski. Qualitative information from multivariate calibration models. Applied Spectroscopy. 44, 1337-1348 (1990).