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Mean centering of double divisor ratio spectra, a novel spectrophotometric method for analysis of ternary mixtures

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ABSTRACT

A novel spectrophotometric method was developed for determination of ternary mixtures without previous separation, showing significant advantages over conventional methods. The new method is based on mean centering of double divisor ratio spectra. The mathematical explanation of the procedure is illustrated. The method was evaluated by determination of model ternary mixture and by the determination of Amlodipine (AML), Aliskiren (ALI) and Hydrochlorothiazide (HCT) in laboratory prepared mixtures and in a commercial pharmaceutical preparation. For proper presentation of the advantages and applicability of the new method, a comparative study was established between the new mean centering of double divisor ratio spectra (MCDD) and two similar methods used for analysis of ternary mixtures, namely mean centering (MC) and double divisor of ratio spectra-derivative spectrophotometry (DDRS-DS). The method was also compared with a reported one for analysis of the pharmaceutical preparation. The method was validated according to the ICH guidelines and accuracy, precision, repeatability and robustness were found to be within the acceptable limits.

1. Introduction

The use of molecular absorption spectroscopy for pharmaceutical analyses has the inherent constraint that most active drugs absorb in the UV region and exhibit strongly overlapped spectra that impede their simultaneous determination. Ternary mixtures suffer a higher degree of difficulty in spectrophotometric resolution than binary mixtures, due to the severe overlap usually noticed in their spectra. Many methods have been developed for resolution of the overlapped spectra of ternary mixtures using different spectrophotometric and chemometric techniques [1–8].

Signal processing techniques have an important role in spectrophotometric resolution of pharmaceutical mixtures, they are more reliable with respect to sensitivity and selectivity than normal spectrophotometry. Several signal processing techniques depend on manipulations of the ratio of overlapping spectra of ternary mixtures. Berzas et al. [9] introduced the derivative ratio zero crossing method for analysis of ternary mixtures, as an extension of the first derivative of ratio spectra method suggested by Salinas et al. [10] which was developed primarily for analysis of binary mixtures. Then Dinç and Onur [11] introduced the Double Divisor of Ratio Spectra-Derivative Spectrophotometry (DDRS-DS) method that was used for the analysis of ternary mixtures. The successive derivative of ratio spectra in two successive steps has been proposed by Afkhami and Bahram [12].

The fact that numerical differentiation degrades the signal to noise ratio (S/N) [13], suggested using other signal processing techniques as powerful alternatives for the analysis of pharmaceutical mixtures. Continuous wavelet transform was applied successfully in zero crossing and double divisor methods for analysis of ternary mixtures [14,15]. Fourier functions were also applied to double divisor method and used successfully for determination of ternary mixtures [16].

Afkhami and Bahram [17] also introduced mean centering as a signal processing resolution tool for analysis of binary and ternary mixtures which involved successive steps of division and mean centering.

In 1998, the Double Divisor Ratio Spectra-Derivative Spectrophotometry (DDRS-DS) method, introduced by Dinç and Onur [11], involved two simple steps for analysis of ternary mixtures. The spectrum of the component of interest was divided by the sum of the standard spectra of the other two components "a double divisor", and then the ratio spectrum was derivatized, where the measurements were done at either maximum or minimum wavelengths. In 1999, Dinç [18] explained that the optimum wavelength for determination is the one at which a coincidence between the spectra of certain concentration of the component of interest and ternary mixture containing the same concentration of this component exists. In his work the coincident wavelengths were at either a maximum or a minimum, and in 2002 higher order derivatives were used to obtain the coincident points at a maximum or a minimum [19]. The method was also faced by the criticism that it cannot be popularized, because it can only be used for mixtures in which the ratio of the concentrations of two interfering compounds (used as double divisor) is known. In other words, the ratio of the concentrations of two interfering compounds should be

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