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Simultaneous Determination of Methotrexate and Aspirin Using Fourier Transform Convolution Emission Data under Non-Parametric Linear Regression Method

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Abstract : Co-administration of methotrexate (MTX) and aspirin (ASP) can cause a pharmacokinetic interaction and a subsequent increase in blood MTX concentrations which may increase the risk of MTX toxicity. Therefore, it is important to develop a sensitive, selective, accurate and precise method for their simultaneous determination in urine. A new hybrid chemometric method has been applied to the emission response data of the two drugs. Spectrofluorimetric method for determination of MTX through measurement of its acid-degradation product, 4-amino-4-deoxy-10-methylpteroic acid (4-AMP), was developed. Moreover, the acid-catalyzed degradation reaction enables the spectrofluorimetric determination of ASP through the formation of its active metabolite salicylic acid (SA). The proposed chemometric method deals with convolution of emission data using 8-points sin xi polynomials (discrete Fourier functions) after the derivative treatment of these emission data. The first and second derivative curves (D1 & D2) were obtained first then convolution of these curves was done to obtain first and second derivative under Fourier functions curves (D1/FF) and (D2/FF). This new application was used for the resolution of the overlapped emission bands of the degradation products of both drugs to allow their simultaneous indirect determination in human urine. Not only this chemometric approach was applied to the emission data but also the obtained data were subjected to non-parametric linear regression analysis (Theil's method). The proposed method was fully validated according to the ICH guidelines and it yielded linearity ranges as follows: 0.05-0.75 and 0.5-2.5 µg mL-1 for MTX and ASP respectively. It was found that the non-parametric method was superior over the parametric one in the simultaneous determination of MTX and ASP after the chemometric treatment of the emission spectra of their degradation products. The work combines the advantages of derivative and convolution using discrete Fourier function together with the reliability and efficacy of the non-parametric analysis of data. The achieved sensitivity along with the low values of LOD (0.01 and 0.06 µg mL-1) and LOQ (0.04 and 0.2 µg mL-1) for MTX and ASP respectively, by the second derivative under Fourier functions (D2/FF) were promising and guarantee its application for monitoring the two drugs in patients' urine samples.

Keywords : chemometrics, emission curves, derivative, convolution, Fourier transform, human urine, non-parametric regression, Theil's method
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