



Univariate vs. Multivariate Calibration in the Quantification of Carbamazepine in Tablets by Raman Spectroscopy using PCA as Spectral Selection Tool

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SUMMARY. When Raman spectroscopy is employed to quantify pharmaceutical compounds, one typically resorts to the multivariate calibration, in order to minimize errors arising from the scattered signal fluctuation. However, molecules of traditional excipients used in tablet formulation emit low Raman scattering, allowing the use of univariate calibration, which is simpler to achieve. In this study, the quantification of carbamazepine in tablets by Raman spectroscopy was performed using univariate and multivariate calibration. To minimize the problem of signal intensity variation, the most representative replicates were selected by Principal Component Analysis (PCA). Univariate and multivariate calibration curves were obtained by simple linear regression and Partial Least Squares (PLS), respectively, resulting in Root Mean Square Errors of Cross Validation (RMSECV) of 4.24 and 3.42 %. The results of this procedure was satisfactory and indicates that with the aid of appropriate numerical treatment, it is possible to perform a simple and reliable method of quantification even when using the univariate approach.

KEY WORDS: Carbamazepine, Partial least squares, Principal component analysis, Raman spectroscopy.

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