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Near Infrared Spectroscopic Transmission Measurements for Pharmaceutical Powder Mixtures

Abstract

Our research describes the development of near infrared (NIR) calibration models using transmission measurements of powder samples, and compares the results obtained with those of tablet transmission and diffuse reflectance of powders. Transmission near infrared spectroscopy is a method widely used for the analysis of tablets in the evaluation of drug concentration due to the larger sample volume analyzed, but not commonly used for the analysis of powder samples. Diffuse reflectance near infrared spectroscopy is used in both powder and tablets for the evaluation of quality attributes of the pharmaceutical products. In this research NIR transmission measurements were obtained using a Bruker Optics Fourier Transform Near Infrared Spectrometer (FT-NIR). Spectra were obtained with three different resolutions for the analysis of powder and tablet samples of 7.50 to 22.50 % (w/w) acetaminophen (APAP) . The Partial Least Squares (PLS) calibration models developed include pretreatments such as Standard Normal Variate (SNV) and first derivative in the region from 9500 to 7500 cm^{-1}. Transmission in powder method presented low Root Mean Square Error of Prediction (RMSEP) values that varied from 0.23 to 1.15 % (w/w) APAP with resolution of 64 and 16 cm^{-1}. The lowest RMSEP values (0.23-0.39 % (w/w) APAP) were obtained using resolution of 64 cm^{-1}. The RMSEP values for powder transmission measurements were 2.35 to 5.61 times lower than diffuse reflectance measurements of the powder mixtures.