Transmission Near-Infrared (NIR) and Photon Time-of-Flight (PTOF) Spectroscopy in a Comparative Analysis of Pharmaceuticals.

We present a comprehensive study of the application of photon time-of-flight spectroscopy (PTOFS) in the wavelength range 1050–1350 nm as a spectroscopic technique for the evaluation of the chemical composition and structural properties of pharmaceutical tablets. PTOFS is compared to transmission near-infrared spectroscopy (NIRS). In contrast to transmission NIRS, PTOFS is capable of directly and independently determining the absorption and reduced scattering coefficients of the medium. Chemometric models were built on the evaluated absorption spectra for predicting tablet drug concentration. Results are compared to corresponding predictions built on transmission NIRS measurements. The predictive ability of PTOFS and transmission NIRS is comparable when models are based on uniformly distributed tablet sets. For non-uniform distribution of tablets based on particle sizes, the prediction ability of PTOFS is better than that of transmission NIRS. Analysis of reduced scattering spectra shows that PTOFS is able to characterize tablet microstructure and manufacturing process parameters. In contrast to the chemometric pseudovariables provided by transmission NIRS, PTOFS provides physically meaningful quantities such as scattering strength and slope of particle size. The ability of PTOFS to quantify the reduced scattering spectra, together with its robustness in predicting drug content, makes it suitable for such evaluations in the pharmaceutical industry.

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