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Traditional versus advanced chemometric models for the impurity profiling of paracetamol and chlorzoxazone: application to pure and pharmaceutical dosage forms

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Abstract

Traditional Partial Least Squares (PLS) and Advanced Artificial Neural Network (ANN) models were applied for the quantitative determination of paracetamol (PAR) and chlorzoxazone (CZX) together with their process-related impurities namely; 4-aminophenol (AP), 4-chloroacetanilide (AC), 4-nitrophenol (NP), 4-chlorophenol (CP) and 2-amino-4-chlorophenol (ACP). Both models were applied first to full spectrum data then the results were compared to those obtained after wavelength selection using Genetic Algorithm (GA). A 5-level 7-factor experimental design was used giving rise to 25 mixtures containing different proportions of the seven compounds. The calibration set was composed of 15 mixtures while 9 mixtures were used in the validation set to test the predictive ability of the suggested models. The four models PLS, ANN, GA-PLS and GA-ANN were successfully applied for the determination of PAR and CZX in their pure and pharmaceutical dosage form. One way ANOVA was carried out between the developed methods and the official ones for PAR and CZX and no significant difference was found. The four models can be easily applied for the determination of the selected drugs in quality control laboratories lacking expensive HPLC instruments.

Keywords: paracetamol; chlorzoxazone; impurities; PLS; ANN; GA