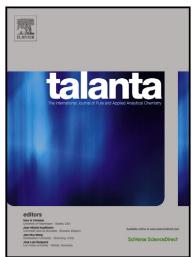
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Combination of electrochemistry with chemometrics to introduce an efficient analytical method for simultaneous quantification of five opium alkaloids in complex matrices

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Abstract

For the first time, an analytical methodology based on differential pulse voltammetry (DPV) at a glassy carbon electrode (GCE) and integration of three efficient strategies including variable selection based on ant colony optimization (ACO), mathematical pre-processing selection by genetic algorithm (GA), and sample selection (SS) through a distance-based procedure to improve partial least squares-1 (PLS-1, ACO-GA-SS-PLS-1) multivariate calibration (MVC) for the simultaneous determination of five opium alkaloids including morphine (MOP), noscapine (NOP), thebaine (TEB), codeine (COD), and papaverine (PAP) was used and validated. The baselines of the DPV signals were modeled as a smooth curve, using P-splines, a combination of B-splines and a discrete roughness penalty. After subtraction of the baseline we got a signal with a two-component probability density. One component was for the peaks and it was approximated by a uniform distribution on the potential axis. The other component was for the observed noise around the baseline. Some sources of bi-linearity deviation for electrochemical data were discussed and analyzed. The lack of bi-linearity was tackled by potential shift correction using correlation optimised warping (COW) algorithm. The MVC model was developed as a quinternary calibration model in a blank human serum sample (drug-free) provided by a healthy volunteer to regard the presence of a strong matrix effect which may be caused by the possible interferents present in the serum, and it was validated and tested with two independent sets of analytes mixtures in the blank and actual human serum samples, respectively. Fortunately, the proposed methodology was successful in simultaneous determination of MOP, NOP, TEB, COD, and PAP in both blank and Download English Version:

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