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Simultaneous identification and quantification of nitro-containing explosives by advanced chemometric data treatment of cyclic voltammetry at Screen-Printed Electrodes

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Abstract

The simultaneous determination of three nitro-containing compounds found in the majority of explosive mixtures, namely RDX, TNT and PETN, is demonstrated using both qualitative and quantitative approaches involving the coupling of electrochemical measurements and advanced chemometric data processing. Voltammetric responses were obtained from a single bare screen-printed carbon electrode (SPCE), which exhibited marked mix-responses towards the compounds examined. The responses obtained were then preprocessed employing Discrete Wavelet Transform (DWT) and the resulting coefficients were input to an Artificial Neural Network (ANN) model. Subsequently, meaningful data was extracted from the complex voltammetric readings, achieving either the correct discrimination of the different commercial mixtures (100% of accuracy, sensitivity and specificity) or the individual quantification of each of the compounds under study (total NRMSE of 0.162 for the external test subset).

Keywords: Electronic Tongue; Artificial Neural Network; voltammetric sensor; explosives; TNT

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