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Electromechanical Chemometrics

Overview

Due to the presence of easily reducible nitro groups, nitroaromatic explosives are inherently electroactive making electrochemical monitoring particularly promising for the construction of highly sensitive and selective explosive sensors. The miniaturization of detection platforms leveraging integrated circuit technology combined with the fast response times associated with voltammetric measurements make electrochemical sensors an ideal candidate for the construction of on-site field deployable devices for detection of explosives.

Approach

In this project, we employed a multivariate approach for the discrimination of similar nitroaraomatic compounds utilizing electrochemical data acquired at a bare glassy carbon electrode (GCE), an aminophenyl-modified GCE, and a carboxylphenyl-modified GCE [1]. As opposed to previous efforts which have primarily relied on separation methods to discriminate chemically similar nitroaromatic compounds, in this study multivariate data analysis methods are employed to extract subtle differences in electrochemical response.

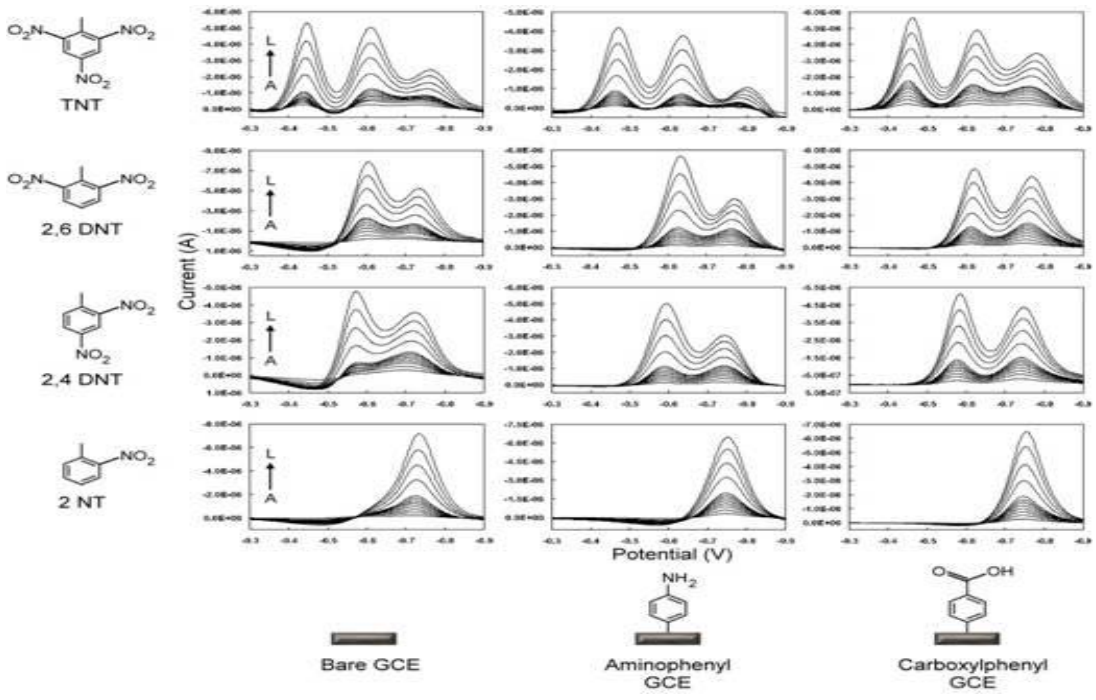

Figure 1. All NT on all surfaces.

The combination of chemometrics, fast voltammetric detection, and selective chemical surfaces could possibly simplify device fabrication by circumventing the need for separation channels and lead to a new generation of on-site field deployable explosive detectors.

The background subtracted electrochemical responses to increasing concentrations of TNT, 2,6-DNT, 2,4-DNT, and 2-NT on the bare, aminophenyl-modified, and carboxylphenyl-modified GCEs are presented below. The number of peaks on each voltammogram corresponds to the number of nitro groups of the respective tri-, di-, and mono-nitrotoluenes. The three different electrode surfaces produce distinct voltammograms which differ in their relative peak potentials and peak currents for each of the four nitroaromatics over the measured concentration range.

Chemometric analysis of this data revealed a strong linear relationship exists between the electrochemical response for the bare GCE, aminophenyl-modified GCE, and carboxylphenyl-modified GCE surfaces and concentrations of TNT, 2,6-DNT, 2,4-DNT, and 2-NT. Additionally, data from the bare GCE, aminophenyl-modified GCE, and carboxylphenyl-modified GCE can successfully differentiate the four different nitroaromatic compounds, as shown in the principal component scores plot below.

References

1. "Multivariate Analysis for the Electrochemical Discrimination and Quantitation of Nitroaromatic Explosives" R. Polsky, C. L. Stork, D. R. Wheeler, W. A. Steen, J. C. Harper, C. M. Washburn, S. M. Brozik, Electroanalysis, 2009, 21, 550-556.

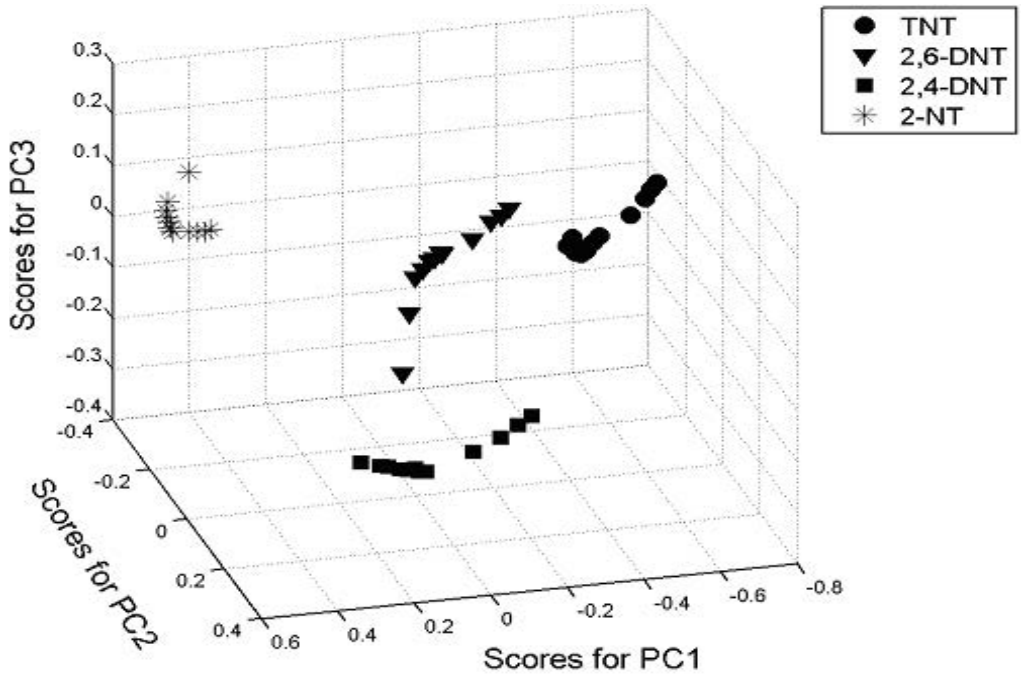

Figure 2. Electrochemical chemometrics.

For additional information or questions, please email us at BioNano@sandia.gov.

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