B49 High-Sensitivity Detection and Separation of High Explosives in Environmental Samples

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The goal of this presentation is to discuss a new technique to detect high explosives in environmental samples using Micellar Electrokinetic Chromatography/Mass Spectrometry (MEKC/MS).

This presentation will impact the forensic science community by examining how forensic chemists can use this rapid and highly sensitive method to separate and identify high explosives in contaminated sand, soil, and water samples.

High explosives constitute the majority of modern military and industrial explosive applications. Because of their wide use, their environmental footprint is becoming an issue. Therefore, identification of high explosives in soil and water is important. Currently, Gas Chromatography/Mass Spectrometry (GC/MS) and High-Performance Liquid Chromatography/Mass Spectrometry (HPLC/MS) are the preferred techniques for the analysis of explosives, yet both have drawbacks. GC/MS is not suitable for the analysis of thermally labile compounds, which include some high explosives, while HPLC/MS lacks sensitivity due to low ionization efficiency of high explosives under negative ionization. Therefore, a selective and sensitive method for the separation and detection of high explosives is desirable. In collaboration with the United States Naval Academy, a novel MEKC/MS technique was developed for the detection of high explosives using a complexation reagent.

Analyses were performed using a Beckman Coulter ProteomeLab™ PA 800 sheathless Capillary Electrophoresis (CE) interfaced to a Thermo™ Orbitrap Elite™ high resolution MS using underivatized fused-silica capillaries (20µm I.D., ~100cm in length) with a porous tip. Electrospray voltage was 1.1kV and the mass spectrometer heated capillary was 150°C. Analyses were performed using a Perfluorooctanoic Acid (PFOA) ammonium salt as a background electrolyte. All samples were injected using pressure (1psi for 4s) and a separation voltage of 25kV was used. Compounds were detected in negative ion mode as a complex with PFOA. Explosive samples from the United States Army Chemical, Biological, Radiological, Nuclear, and Explosives (CBRNE) Analytical & Remediation Activity Mobile Expeditionary Laboratory have been obtained, extracted, and analyzed using this newly developed MEKC/MS method.

High explosives that formed complexes with PFOA included RDX, HMX, tetryl, and PETN. Also, amino-dinitrotoluene formed a complex with PFOA. Other nitroaromatics were detected as molecular ions. The five explosives which formed complexes with PFOA had detection limits in the high parts-per-billion range and linear calibration responses over two orders of magnitude. The technique was successfully applied to the quantitative analysis of high explosives in sand samples.

Using PFOA as a background electrolyte, high explosives from contaminated sand samples could be separated and detected with high sensitivity.

High Explosives, Environmental Samples, CE/MEKC/MS

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