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# Explosives Analysis using Gas Chromatography/Mass Spectrometry

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The goal of this presentation is to discuss the analytical challenges associated with the identification of high explosive compounds along with some practical solutions to these problems. The goal of this research is to produce a GC/MS database containing consistent and unique mass spectra for the high explosive compounds.

After this presentation, the attendees will be able to assess their current laboratory techniques (if any) for the analysis of these problematic compounds and determine if the GC/MS method presented will improve trace explosives identification for a wider variety of compounds in relation to their current methods.

This research will benefit the forensic science community by showing laboratory personnel how to adjust their GC/MS equipment for the clearest mass spectra of high explosive compounds and their isomers. This research will demonstrate what compounds to identify for the high explosives that do not survive typical GC/MS. It also presents the community with a new database of compounds for the GC/MS including common high explosives and related compounds. Such a complete database of these compounds is difficult to find making this a useful tool for any laboratory.

More labs use GC/MS than any other technology for analytical purposes. Gas chromatography (GC) is advantageous in trace analysis as it has a high resolving power, resulting in more efficient separations, which lead to better identifications. Mass spectrometry (MS) is an accurate and reliable detector with the capability of examining a broad range of compounds and identifying them with specificity. The combination of GC with MS allows for improved separation of complex matrices and specific identification of trace analytes.

The greatest obstacle when identifying high explosive compounds by GC/MS is their high reactivity and propensity to decompose rapidly at high temperatures. At the wrong temperatures the explosive compounds decompose and their mass spectra contain ions that can be found in a wide variety of molecular decompositions making it difficult to produce and identify a unique explosive compound. In addition to the temperature challenges, active sites can be found throughout the chromatographic system attracting these explosive compounds and binding with them. The explosive compounds become lost in the system and never appear in the MS source to produce a spectrum.

This research will benefit the larger community of law enforcement, military and even industry by providing more options to laboratories for explosive analysis. Forensic explosive analysis can identify compounds in improvised explosive devices (IEDs) and land mines in war zones to properly identify explosive components in post detonation situations. This data can also be used to assist in identifying a suspect as well as detecting live IEDs or land mines for disarming. Explosive manufacturers and research facilities would benefit from improved analytical techniques to determine the quality of their product and to evaluate changes that occur to bulk materials in storage.

The benefits go beyond these communities, however, extending into the environmental and medical fields. Many explosive compounds are highly toxic to animals and humans under long periods of exposure. Long-term exposure to TNT, for instance, can cause blood disorders, liver and spleen failure, decreased immune response, and cataracts. Improved analysis will help identify environmental soil and water samples contaminated by runoff and erosion from blasting and storage sites at lower levels so the problem can be remedied before permanent damage can occur. Along with

proper extraction techniques, GC/MS is capable of isolating and identifying each specific compound at the trace levels these compounds will most likely appear.

The authors will present on the challenges associated with this research project, our solutions to those challenges, and the resulting mass spectra for high explosives and related compounds for compilation into a user-searchable database.