## A9 Statistical Discrimination of Explosive Precursors Using Data Gathered From High Resolution Fourier Transform Infrared Spectroscopy

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The goal of this presentation is to give attendees an understanding of the statistical analysis used to discriminate between potential explosive precursor materials based upon spectra produced using highresolution Fourier Transform Infrared (FTIR) spectroscopy.

This presentation will impact the forensic science community by demonstrating the use of readily available statistical software to discriminate between similar infrared spectra, initially applied to the analysis of explosive precursors, but with the potential for use in other areas of forensic analysis.

The characterization and discrimination of different explosive precursors is an integral part of the information gathering used in the development of explosives detection security systems. Detection of precursors facilitates the interception of such materials prior to the completion of an explosive device. The ability to discriminate between explosive precursors of different origins facilitates accurate detection, providing greater strength of evidence against suspected bomb-makers.

The increased use of the so-called “homemade explosives” has resulted in a range of potential explosive precursors. As the name suggests, these explosive materials can be produced without a specialist laboratory from precursor materials that are easily purchased in small amounts. However, the precursor materials are often not in a pure form depending on their commercial purpose. For example, acetone is the active ingredient in many nail polish removers and it is combined with emollients, conditioners, perfumes, and colorants to enhance the product. Different brands with different ingredients have the potential to produce different infrared spectra, thereby giving the potential for discrimination. Depending upon the concentration of the primary ingredient, its spectrum may be masked by the other ingredients. In addition, many explosive precursor materials in their “off the shelf” form contain a relatively large amount of water, which also affects the infrared spectrum. Through previous work, highresolution FTIR spectroscopy has been demonstrated to be suitable for the characterization of laboratorygrade explosive materials and their precursors, as the technique produces information-rich spectra. The production of information-rich spectra helps to overcome the issues of masking and water interference. Discrimination may be possible from visually examining spectra of different precursor brands; however, statistical techniques can be used to detect minute differences between spectra which on the surface appear visually very similar. Moreover even in cases where the spectra appear visually different, statistical analysis can aid the discrimination of different “off the shelf” brands.

Three main statistical techniques were used to explore the best data mapping system for the complex data emerging from the analysis: cluster analysis, principal component analysis, and, Pearson correlation. The data presented here detail the development of a protocol for the stepwise application of data processing, followed by statistical analysis for the discrimination of explosive precursors and the initial results obtained from the application of the protocol.

**Statistics, Cluster Analysis, Explosives**

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