A183 Development and Validation of AccuTOF- DART(TM) as a Screening Method for Analysis of Bank Security Device and Pepper Spray Components

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After attending this presentation, attendees will be familiar with the results of the validation for a method of screening for pepper spray and bank security device components using Direct Analysis in Real Time (DART^{TM}) ionization coupled with Accurate Time-of-Flight (AccuTOF) mass spectrometric detection.

This presentation will impact the forensic science community by providing a much more efficient procedure for processing evidence of this type by decreasing the time spent analyzing negative samples and by quickly identifying areas of interest on positive samples.

Currently at the Virginia Department of Forensic Science, cases involving pepper spray and bank security devices are analyzed similarly. An initial visual screen is performed to locate noticeably stained areas. The visual screen is more effective in the case of bank security devices due to the red dye, 1-methylaminoanthraquinone (MAAQ), which is contained in these devices. However, a visual scan may not locate stains on darkly colored clothing and can not determine the source of the red color. Pepper sprays can be difficult to locate visually due to capsaicin's, the main component in such sprays, lack of color. Visual screens can be aided by the use of UV light, but this method has no specificity and many stains can still be missed. Stained areas are extracted for confirmation of MAAQ, o-chlorobenzylidenemalononitrile (CS, a tear gas), or capsaicin by GC/MS. When no stains are visible, a random sampling of areas is extracted for GC/MS analysis, which can be very time-consuming.

This study consisted of five main steps: (1) Optimization of AccuTOF-DARTä parameters for each analyte; (2) Determination of the most efficient extraction solvent for each analyte; (3) Development of an appropriate technique for introducing fabric samples into the DARTä sample gap; (4) Development of an appropriate technique for extracting samples for GC/MS confirmation; and, (5) Validation of the final method by determining the lower limit of detection (LLOD) of the method, interferences, selectivity, reproducibility, and robustness.

For the optimization of parameters, each analyte was tested at a range of different temperatures and orifice 1 voltages to determine the most favorable conditions for ionization and detection. A gas temperature of 325°C was chosen for all analytes. The first voltage provides a spectrum showing protonated molecules while the second voltage provides additional spectral information via collision induced dissociation. For MAAQ and CS, orifice 1 voltages of 30V and 85V were chosen, while 20V and 50V were best for capsaicin. To determine the appropriate extraction solvents, each analyte was spiked onto several different fabrics and extracted with hexane, dichloromethane, and methanol and analyzed on the GC/MS. Hexane was found to be iDrug Enforcement Administrationl for MAAQ and CS, while methanol was best for capsaicin. The main focus of this research was the determination of an appropriate sampling technique for fabrics on the AccuTOF- DARTä. Inserting the stained fabric directly into the DARTä sample gap

was the simplest and most efficient technique, but several problems arose with some fabrics melting in the high gas temperature or introducing lint into the ion optics of the AccuTOF. The best technique was found to be extraction through the fabric onto cardstock followed by direct insertion of the stained cardstock into the DARTä sample gap. Methanol was chosen as the extraction solvent for all analytes due to its added screening ability of maintaining the red color of MAAQ, while hexane produced a pale yellow extract that was not readily visible on the cardstock. After AccuTOF-DARTä screening, stains were cut from the cardstock and extracted in hexane for MAAQ and CS or methanol for capsaicin, followed by concentration of the extract prior to confirmation by GC/MS. The LLOD of the method was determined by spiking fabric samples with serial amounts of each analyte and analyzing with the final method. No spectral interferences were found for any of the analytes. No potential selectivity issues were determined for MAAQ or CS. Pepper sprays were tested alongside hot sauces, which also contain capsaicin, to determine a method for differentiation between the two. Differences were found in the relative abundance of the ion peak representing linoleic acid vs. the ion peak representing capsaicin. The linoleic acid peak is relatively large compared with the capsaicin peak in hot sauces, whereas it is insignificant compared with the capsaicin peak in the pepper sprays tested. Reproducibility was determined by repeating the LLOD studies ten times each on two different days. Robustness was shown by having three separate analysts repeat the LLOD determination for each analyte.

The combination of sample extraction onto cardstock followed by analysis using AccuTOF-DARTä can provide an efficient method for analyzing evidence for the presence of bank security device components and pepper spray components, saving time both in the location of such stains and in the early elimination of negative samples. This study validates the use of the AccuTOF-DARTä in such an analysis scheme. **Direct Analysis in Real Time, Pepper Spray, Bank Dye**

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