K30 Identification of Product Adulteration With Pesticides Via Direct Analysis in Real Time (DART™) Time-of-Flight Mass Spectrometry (TOF-MS)

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The goal of this presentation is to demonstrate that DART-TOF-MS instrumentation is a beneficial counterpart in the modern forensic laboratory to traditional toxicological examinations.

This presentation will impact the forensic science community by demonstrating how Direct Analysis in Real Time (DART) ionization sources may provide a more rapid and direct analytical route to toxicant identifica- tion in adulterated food or beverage specimens.

DART™ stands for "Direct Analysis in Real Time". A new ion source, DART™ allows for the direct detection of chemicals on surfaces, in liquids, and in gases without the need for sample preparation. The ion source is open to the atmosphere, and does not require a vacuum, the use of high voltages or solvent sprays. Samples are simply placed into the ionization stream. The ionization mechanism is based upon the reactions of excited-state species with reagent molecules and polar or non-polar analytes. When coupled with a TOF-MS, accurate mass assignments are generated and analyte identifica- tions are realized.

In many toxicological investigations, the suspected source of the poison may be received in addition to biological specimens such as blood or urine. Often, the most direct route to toxicant identification is primary analysis of suspect source material. However, analysis of seized food, beverage, and other commercial products is typically time consuming and laborious. A DART-TOF-MS instrument offers the forensic examiner a tool for rapidly identifying such adulterations in bulk samples. Such analyses can complement subsequent traditional investigations by immunoassay and chromatography.

Several cases are presented in which beverages or food products were suspected to have been spiked with a commonly available pesticide formu- lation. Commercially available herbicide formulations often contain a variety of organochlorine, organophosphorus or other compounds. Ingestion of such preparations may cause severe injury or death.

Direct analysis of both the seized food samples and a pesticide exemplar by DART-TOF-MS yielded a rapid and conclusive identification. The analysis provided exact molecular mass, theoretical isotope distribution matching, and characteristic fragmentation patterns to effect the identifica- tions. No sample preparation was required. The pesticides identified were 2,4-D, dicamba, mecoprop, and diethyltoluamide.

DART-TOF-MS, Pesticides, Accurate Mass

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