

Papers Presented at Pittcon 2007 Relevant to JEOL AccuTOF-DART™

"PITTCON: The Development of a Searchable Commercial Products Library for DART Spectra"

Presented by: Lisa Schumacher, Federal Bureau of Investigation, 2501 Investigation Pkwy, Quantico, VA 22135, Brenda Vaandering, Eshwar Jagerdeo, Jamelle Williams, Jay Clark, Jeff Leibowitz

Abstract: The DART is one of the greatest advances in technology in our fight against crime. It offers real-time analysis of evidence as it was discovered by law enforcement officers in the field generating exact-mass measurements and patterns which are then used for identification. The DART system is composed of an ionization source that uses Helium in its excited state to ionize a sample that is placed in the gas stream and an accurate mass time-of-flight mass spectrometer to detect the ions produced. This direct analysis in real-time (DART) method of ionization is most similar to electrospray ionization and usually, but not always, generates M+1 or M-1 ions. But unlike electrospray, analysis by DART generates a pattern instead of a single peak because there is no separation of a sample into its individual components - like with gas chromatography or liquid chromatography - prior to entering the mass detector. The DART is essentially generating a unique picture (mass spectrum) of numbers (exact masses) and lines (pattern) to represent the components in a specific sample, like the ingredients in a commercial product. For example, the analysis of two different soft drinks would generate two very unique pattern-specific mass spectra that could be used to narrow the identification of an unknown brown liquid received by the laboratory as having ingredients consistent with a soda but also differentiate between the two and positively identify it as Brand X. As this technology is new, however, there are no databases or libraries in existence to search DART® spectra against to identify commercial products. The FBI is currently working to develop and populate a searchable Commercial Products Library.

"PITTCON: Additional Real Time Structural Information"

Presented by: Patrick Jones, University of the Pacific, 3601 Pacific Avenue, Chemistry Department, Stockton, CA 95211-0001, Changnan Chen, O. David Sparkman, Robert B. Cody, Teresa Vail

Abstract: The Direct Analysis Real Time, DART, interface on a TOF MS instrument has been shown to provide accurate mass, in-source CAD fragmentation, and isotope pattern matching for rapid identification of a wide range of materials. We report a fourth source of structural information is available by in-source hydrogen-deuterium exchange reactions. The number of exchangeable hydrogens on a target molecule can be counted without pretreatment of the original sample. Amino acids provide an example of species detected in dilute solution from the residue that adheres to a glass rod dipped into the solution with DART MS spectra that show all four types of structural information. These data and data of other compounds with exchangeable hydrogens will be presented. A unique apparatus for obtaining these data will also be presented.

"PITTCON: A \$250 Autosampler for a DART Ion Source and Deconvolution of Composite Mass Spectra Based on Exact Masses and Relative Isotopic Abundances"

Presented by: Andrew H. Grange, U.S. Environmental Protection Agency, Environmental Chemistry Branch, PO Box 93478, Las Vegas, NV 89193, Wayne Sovocool

Abstract: Chemicals are dispersed by numerous accidental, deliberate, or weather-related events. Often, rapid analyses are desired to delineate areas of contamination and to identify dispersed chemicals. Hundreds of wipe samples might be collected from building interiors or outdoor surfaces both before and after any remediation. A DART/oa-TOFMS analyzes

compounds in ambient air in seconds on surfaces such as a cotton swab without requiring extraction, extract clean-up, or chromatography. The open design of the ionization region enabled construction of a simple, \$250 autosampler based on N-scale model railroad components and 3' x 1/4"- square aluminum rods. Holes spaced 15/32" apart for cotton swabs through each of 14 rods provide for analysis of 1000 samples. Using a rod as the core of a field sampling fixture to provide cotton swab wipe samples that are almost ready for analysis upon receipt might enable one analyst to **perform 1000 analyses in one 8-hour shift.** In addition, an in-house Ion Correlation Program (ICP) has been used to deconvolute composite mass spectra from multiple analytes on a single cotton swab based on exact masses of monoisotopic ions and the relative isotopic abundances of their +1 and +2 isotopic peaks rather than on the retention time differences of ions provided by chromatography. After mass spectral deconvolution, each of several compounds was identified from its elemental composition. The autosampler, integrated field sampler/autosampler, ICP, and preliminary data will be described.