C15 Semi-Quantitative Mapping and Identification of Dispersed Chemicals Using an Ambient-Air Ion Source/ Mass Spectrometer

Andrew H. Grange, PhD, United States Environmental Protection Agency, Environmental Sciences Division, PO Box 93478, Las Vegas, NV 89119*

The goal of this presentation is to inform attendees about a new, high throughput, highly specific analytical technique for identifying and mapping dispersed chemicals.

This presentation will impact the forensic science community by leading to more thorough characterization of contaminated sites, real- time monitoring of remediation, and documentation of thorough clean-ups.

The research focus is to develop high throughput analyses to semi- quantitatively map with high spatial resolution polar chemicals dispersed accidentally, deliberately, or by weather-related events or present in Superfund or Brownsfield sites. Recently developed ambient-air ion sources provide highly specific, mass spectral analysis of compounds adsorbed on surfaces in several seconds. Development of an autosampler and field sample collection system could provide 10-100 times faster analyses than conventional mass spectrometric methods, thereby greatly reducing analysis costs and enabling more rapid and thorough characterization of contaminated areas. A Direct Analysis in Real Time (DART®) ion source directs a heated and energized helium stream onto surfaces to desorb and ionize analytes absorbed on surfaces. The ions are analyzed by a Time-of-Flight Mass Spectrometer (TOFMS), which measures exact masses and relative isotopic abundances that provide the elemental compositions of ions and a compound's identity. Because time-consuming chemical separation techniques are not used, software was written to deconvolute composite mass spectra based on the exact masses and relative isotopic abundances of the ions from multiple compounds. An autosampler was designed, built, and tested that incorporated N-scale model railroad flatcars, track, and a transformer (±15 VDC power supply); a 3-feet-long, 1/4-inch-square bar; fish line; a small 7-rpm motor; and other easily procured and inexpensive parts. Cotton swab wipe samples were inserted through holes in the bar spaced ½ inch apart. In 7.5 minutes, 76 cotton swab wipe samples were analyzed. To provide wipe samples to the lab nearly ready for analysis and to simplify sample collection, a field sample carrier was built around the aluminum bar. Only five minutes was required for sample preparation for each set of samples. The cost of materials for the two devices was about $350. To determine the feasibility of plotting a semi-quantitation map for an analyte, ten NoDoz® (45% caffeine) tablets were ground to powder and dispersed across a concrete driveway using a shop vacuum operated as a blower. A four-color, semi-quantitation map for high, moderate, low, and non- detect levels of caffeine was plotted from the abundances for the m/z 195 $[M+H]^+$ ion from the analyte. The wipe samples were collected from a 7 x 12 sampling grid by dipping the cotton head of a 6-inch swab into water and then rolling it back and forth from side to side and from top to bottom within a 10-cm square template. Palliatives for analyte carryover between swabs during the analyses were use of water-soaked swabs interspersed between the analyte swabs to generate hot water vapor that washed condensed analyte from the inlet orifice cone into the mass spectrometer and signal integrating software that accounted for the remaining carryover. Other sampling techniques are being developed to sample soil, sand, and grass surfaces that will provide an aqueous extract within a few minutes into which a cotton swab will be dipped. Successful development of additional sampling techniques will provide a high throughput analytical technique for rapidly mapping contaminated areas, for locating "hot spots" in Superfund and Brownfields sites, for guiding remediation in real time, and for documenting thorough clean up of contaminated sites. Rapid mapping of contaminated sites with high spatial resolution will provide better risk assessments for humans and ecosystems and better delineate contaminated areas in need of remediation.

Dispersed Chemical, Rapid Analysis, Mass Spectrometry

** Presenting Author*