A94 DART®-AccuTOF™ as a Complementary Tool, or is it an Essential Tool in Managing Today's Complex Drug Chemistry Environment?

Erin M. Shonsey, PhD, Vaughn Barron, MEd, Andrea Headrick, BS, and Dale Carpenter, PhD, Alabama Department of Forensic Sciences, 2026 Valleydale Road, Hoover, AL 35244*

After attending this presentation, attendees will learn the need for additional screening techniques in controlled substances analysis for robust case analysis.

This presentation will impact the forensic science community by investigating and filling a void in current controlled substances analysis, greatly reducing the risk of false negatives.

Whether we are cognizant of it or not, there exists a void in the classical screening capabilities of conventional drug chemistry laboratories. For the majority of cases encountered by forensic chemists, analysis with traditional methodologies is sufficient. However, the controlled substances world is not static, and the increasing complexity of not only controlled substances but also product tampering cases, is outpacing the capabilities of classical analytical techniques. Introduction of newer technologies into the classical workflow is essential to keep pace with the controlled substances world. The introduction of the DART®- AccuTOF™ has increased screening capabilities in a single analysis by orders of magnitude in a fraction of the time.

The DART® is one of the first open air, ambient pressure ion sources for a mass spectrometer. The design of the DART® opens the source for sampling substances in either solid, liquid, or gas states. This simplifies the sample preparation and extraction prior to analysis. In most instances, no sample preparation is required, and in fact, the raw sample is preferred for analysis. Analysis of a variety of substances including unknown powders, residues, organic liquids, plant materials, and aqueous liquids is possible without any sample preparation or extraction. The combination of the DART® with an AccuTOF™ mass spectrometer provides putative identifications of compounds based on molecular mass measurements. This process is targeted for analysis of protonated molecular ions, or $[M+H]^+$ ions, resulting in a mass spectrum of the analytes that are capable of being ionized. This means that the intact mass of a compound must be measured within five millimass units (mmu) of the theoretical mass based on molecular formula for a positive screening result.

Drug Chemistry workflow in the laboratory consists of presumptive and confirmatory testing. Traditional presumptive tests include color tests, microcrystal tests, and gas chromatography or liquid chromatography analysis. Mass spectral identification is required for controlled substances confirmation in many laboratory systems. The void

became readily apparent with the implementation of the DART®- AccuTOF™ into the screening process utilized in the author's laboratory. As a result the workflow was changed to require DART®-AccuTOF™ screening prior to a conclusion that no controlled substances are detected. This applies to approximately 5% of the cases encountered in the author's laboratory system. Cases which screen positive by DART®- AccuTOF™ analysis undergo further testing to determine if molecular identification is possible.

Since the adoption of the DART®-AccuTOF™ screening, a suprising 40% of the cases (2% of the total) analyzed in the complementary workflow have screened positive. The cases that screened positive underwent additional analyses and mass spectral identification was obtained for controlled substances approximately 50% of the time or in 1% of the total cases analyzed. The ability to direct the analysis prior to extraction with a screening tool that covers the wide range of samples encountered in the laboratory has increased the ability to detect and confirm controlled substances. It has therefore been determined that the DART®-AccuTOF™ has become an essential tool for case analysis (demonstrating superiority to GC/MS in determination of true negatives), evaluation of extraction efficiency, and method development within the Alabama Department of Forensics Drug Chemistry laboratories.

Controlled Substances, DART®-AccuTOF™, New Technology

 ** Presenting Author*