K10 DART-TOF Applications in Toxicology and Controlled Substances

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After attending this presentation, attendees will be aware of applica- tions for Direct Analysis in Real Time – Time of Flight Mass Spectrometry (DART-TOF) in the disciplines of toxicology and controlled substances. These applications were based on observations from data collected from casework and in the creation of user libraries. These libraries are comprised of pure compounds, analytes in solution and pharmaceutical preparations.

This presentation will impact the forensic science community by providing sample data and user libraries on a relatively new instrument so that forensic laboratories can understand how this new instrumentation could assist forensic laboratories in casework production.

DART-TOF is a novel technique that allows for the quick identifica- tion of target analytes. DART is unique ionization source in that it uses an open air sampling interface for rapid sampling and that enables the TOF-MS to provide real time mass spectrometry data. The selectivity of the instrument is based upon the high degree of mass accuracy and the fragmentation observed at high voltages. The DART-AccuTOF© instrument used was created by and purchased from JEOL.

In the discipline of controlled substances, the purpose of DART is to improve the efficiency of the identification of controlled substances, thus increasing the output production of the laboratory. Case samples were analyzed to evaluate the ability of this instrument to meet this objective. Concurrently, a library of over 400 controlled and non-controlled substances was constructed and compared to calculated masses found in the literature.

The types of samples currently being evaluated are Marihuana and pharmaceutical preparations. For Marihuana, it is important to be able to distinguish ∆9-Tetrahydrocannabinol and Cannabidiol in order for this instrument to be considered a conclusive examination for this substance. These two compounds have identical molecular formulas and can not be distinguished without fragmentation. This fragmentation was observed at higher voltages and different ionization modes. Signature fragments are being evaluated to distinguish compounds from one another when possible. Compounds that are potential interferences and have the same molecular weight as ∆9-Tetrahydrocannabinol was evaluated for their signature fragments.

Pharmaceutical preparations are an ideal candidate for quick analysis due to the fact the imprinted logo presumptively identifies which compounds are present, both controlled and non-controlled. Two compounds of interest due to the frequency of submission to the laboratory are codeine and hydrocodone. These compounds have identical molecular formulas and these compounds are being evaluated to determine how they can be distinguished by their signature fragments. A tablet library was also being constructed so that tablets from specific companies could be identified not only by their primary compound, but also by the ratio of inactive and inert ingredients.

In the discipline of toxicology, DART-TOF can be used to examine gastric contents and tablets found in gastric contents. Results from the analysis of toxicological specimens analyzed by DART-TOF will be presented.

DART, Controlled Substances, Toxicology

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