A140 Determination of Useful Yields of Forensically Relevant Compounds by Direct Analysis in Real Time Mass Spectrometry (DART/MS)

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After attending this presentation, attendees will be familiar with the concept of useful yields and their relevance to the forensic community, while also discussing the topics of useful yields for a number of forensically related compounds, including explosives, narcotics, bank dye, and lubricants.

This presentation will impact the forensic science community by giving an in-depth understanding of useful yields and how they can be improved to better understand the limit of detection and limit of quantification of mass spectrometry analysis. Furthermore, the effects which instrument parameters have on the useful yields of the compounds will be explored. Comparison of the useful yields of the DART®-MS technique to other mass spectrometry techniques will also be discussed.

Useful yield is a term which is not widely used in the Ambient Pressure Ionization Mass Spectrometry (API-MS) realm. It has; however, been utilized in the Secondary Ionization Mass Spectrometry (SIMS) area of study. The definition of useful yields is the ratio of the ionized molecules to the amount of molecules originally present in the sample. This measurement allows for a way to measure the efficiency and practical yields of a given substance through analysis on a specific technique with specific settings. Useful yields can also be used to compare two techniques which are difficult to compare otherwise. By understanding the useful yields it may be possible to determine which technique would provide the best response for a given analyte or class of analytes.

To obtain a useful yield, it is crucial to have a precise understanding of the number of analyte molecules present in the sample. In order to obtain an accurate number, two methods of sample deposition can be used. The first method is a microsyringe, which will deposit a relatively accurate amount of analyte to a substrate. The second and more precise technique is piezoelectric inkjet printing, which allows for the printing of microdroplets of solution onto a surface. Using this technique, it is possible to obtain 1% repeatability and ±10% accuracy in sample deposition.

Useful yields were determined for a number of compounds on an AccuTOF™ DART® mass spectrometer. The DART® source is a commercial-available API-MS technique which is gaining momentum for routine use in casework, and, therefore, is a prime technique for this study. Since there are several different parameters which affect the signal, the useful yields under a number of different parameters were studied. These parameters include gas temperature, orifice voltage, and the addition of a dopant. How much of these factors influence the useful yield is discussed. The analytes which are examined include explosives, narcotics, bank dye, and lubricants. Initial results on the useful yields of explosives show that about one in every 10^8 – one in every 10^9 molecules are ionized and detected. This compares closely to results for other API-MS techniques, including Desorbtive Electrospray Ionization (DESI) and Low Temperature Plasma (LTP). Useful yields from DART®-MS are also compared to both vacuum-based techniques and chromatographic techniques such as SIMS and GC/MS.

DART®-MS, Useful Yields, Explosives

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