A162 Rapid Analysis of Multiple - Unit Exhibits Using Mass Spectrometry: No Chromatography Necessary

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After attending this presentation, attendees will have knowledge of the recently developed techniques of ESI, APCI and DESI, and their used during forensic chemistry casework.

This presentation will impact the forensic community by increasing awareness regarding new state-of-the-art analytical techniques of great used to the criminalistics community.

The development of the soft ionization technique of electrospray ionization (ESI) during the mid eighties extended the application of mass spectrometric (MS) techniques to the analysis of large, polar, non-volatile molecules. During the last 20 years, applications of ESI and other atmospheric pressure ionization (API) techniques have exploded and these days the use of LC-MS instrumentation is relatively common in academia and the pharmaceutical industry. However, the adaptation and utilization of these techniques in forensic laboratories has been slower, as the traditional technique of choice for MS analysis is usually gas chromatography–mass spectrometry (GC-MS). In this presentation, the advantages and limitations of ESI, atmospheric pressure chemical ionization (APCI) and desorption electrospray ionization (DESI) will be discussed. Examples will be presented demonstrating the successful use of ESI-MS/MS, APCI-MS/MS and DESI-MS/MS experiments during the screening of multiple-unit exhibits.

ESI and APCI are the two most common ionization interfaces used during routine liquid chromatography - mass spectrometry (LC-MS) experiments. During ESI, ions in solution are transported into the gas phase via a series of solvent evaporation and Coulomb explosion events. Greatly influenced by solution chemistry properties, the softness of the ESI process allows the detection of intact compounds as singly or multiply protonated ions of the form $(M+nH^+)^{n+}$. For APCI, ionization solely occurs via single protonation of the analyte based on its gas-phase chemistry. Both ionization techniques, when interfaced to a mass spectrometer, provide molecular weight information and allow the use of collision induced dissociation (CID) experiments for structural elucidation. Ionization via ESI is ideal for the analysis of polar controlled substances, while APCI is more amenable for the study of compounds of intermediate or low polarity, like anabolic steroids and cannabinoids.

DESI is one of the most recently developed ambient ionization techniques, where samples can be analyzed either directly or after deposition onto a non-conducting surface. An extension of electrospray, DESI allows the rapid screening of tablets, liquids, and plant material without the need for sample preparatory steps. Analytes are also detected as protonated species providing molecular weight and structure information via MS experiments.

In this presentation, presumptive and confirmatory MS methods using ESI, APCI and DESI will be presented. Examples will include ESI- MS analysis of opium, ESI-MS/MS analysis of methamphetamine and heroin bulk exhibits, ESI-MS/MS/MS analysis of cocaine samples, APCI- MS analysis of testosterones, APCI-MS/MS analysis of nandrolone decanoate, DESI-MS and DESI-MS/MS analyses of single and multi-component tablets.

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