B75 Forensic Applications of Liquid Chromatography Mass Spectrometry (LC-MS)

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The goal of this paper is to present applications of LC-MS in the forensic chemistry laboratory.

This presentation will impact the forensic science community by demonstrating the use of LC-MS for routine forensic analysis.

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 ionization 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 mass spectrometric identification is usually gas chromatography – mass spectrometry (GC-MS). During this presentation, the principles and applications of LC-MS in the forensic chemistry laboratory will be discussed.

The presentation will include a discussion of the atmospheric pressure ionization techniques of ESI and APCI. Many laboratories and forensic chemists are very familiar with the principles and applications of electron ionization (EI) as it is used in commercial GC-MS instruments. Similarities and important differences between this ionization technique and the soft ionization techniques used during LC- MS will be discussed. In addition, significant differences between GC- MS and LC-MS instruments will be addressed.

Electrospray ionization allows for the analysis of a wide variety of compounds by producing singly or multiply charged pseudo-molecular ions that can be transported from solution into the gas phase with minimal fragmentation. Highly basic compounds like phenethylamines and natural alkaloids are easily ionized, and analysis via ESI produces intact pseudo-molecular ions that provide molecular weight information, often absent in GC-MS data. Further analysis of such pseudo-molecular ions via fragmentation or collision induced dissociation (CID) experiments provides for confirmatory identification of unknown compounds, either by interpretation of fragmentation patterns or by comparison with reference standards.

This presentation will also include the discussion of LC-MS qualitative methods for the analysis of phenethylamines, tryptamines, cocaine, heroin, and other controlled substance exhibits. Direct injection (non-LC) applications will also be discussed, as they provide a way to perform rapid screening and analysis of multiple-unit exhibits and purified standards. The use of ESI-MS for monitoring the synthesis of clandestinely manufactured compounds will also be presented.

Additional discussion and examples will include the use of the recently developed technique of desorption electrospray ionization (DESI) mass spectrometry for the rapid screening of tablets, plant material, THC-containing exhibits, opium, and cocaine base samples. The use of APCI during the analysis of steroids, GHB, GBL, and 1,4- butanediol will also be illustrated.

LC-MS, Electrospray, Controlled Substances

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