B162 Separation and Identification of Drugs of Abuse by nano-Liquid Chromatography/Electron Ionization/ Mass Spectrometry (nLC/EI/MS)

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After attending this presentation, attendees will understand the merits of nLC/EI/MS for the analysis of drugs of abuse when compared to Gas Chromatography/Mass Spectrometry (GC/MS) and Liquid Chromatography/ Electrospray Ionization/Tandem Mass Spectrometry (LC/ESI/MS/MS) methods.

This presentation will impact the forensic science community by introducing a viable method for the separation and identification of thermally labile drugs of abuse, as well as the advantages of nLC/EI/MS when compared to GC/MS and LC/MS/MS.

GC/EI/MS and LC/ESI/MS/MS are two commonly used analytical techniques in the forensic analyses of drugs and explosives. The primary advantage of GC/MS is its extensive library-searching capability, which allows identification of unknown compounds; however, many compounds used in forensic sciences are thermally labile and decompose in the GC injector, which typically operates at high temperatures. LC/MS has been useful in addressing the issue of thermal degradation by utilizing an atmospheric pressure ionization source, such as ESI, eliminating the need for a high-temperature injector and, therefore, vastly decreasing or eliminating fragmentation.[1] By using an MS/MS, compounds can be fragmented; however, no good library for LC/MS/MS currently exists.

LC/EI/MS is an ideal analytical technique for the analysis of thermally labile drugs because it combines the advantages of the LC for sample introduction at low temperatures with the EI/MS ionization, fragmentation, and library-searching capability.[2] Many Novel Psychoactive Substances (NPS), including synthetic cathinones and synthetic cannabinoids, are thermally labile and, therefore, are difficult to detect and identify using GC/MS. Moreover, analysis of these compounds by LC/MS/MS is hindered by the lack of a universal library searching of the MS/MS spectra. There is also a need to develop a field-portable analytical technique for on-site real-time confirmatory analysis of illicit drugs, especially the synthetic drugs that are flooding the illegal markets. To address these issues, a field-portable nLC/EI/MS is being developed by using a field-portable Easy 1000 nanoLC™ in conjunction with a field-portable Viking 573 mass spectrometer, on loan from the Federal Bureau of Investigation (FBI). Development of the nLC/EI/MS also allows the analysis of thermally labile compounds or compounds that are difficult to analyze by GC/MS. NanoLC flow rates are in the range of 100nL-500nL/min, allowing the sample to be introduced directly into the MS ion source. Analytes are then ionized and fragmented using electron ionization, producing fragmentation patterns similar to the conventional GC/MS. An nLC flow rate of 300nL/min was used with a mobile phase of H_2O and acetonitrile each containing 0.1% formic acid. First, the method parameters such as flow rate, column length and inner diameter, mobile phase composition, and injection volume were optimized for maximum sensitivity using caffeine, methamphetamine, and morphine. After determining the optimum parameters, a nano C18 column was attached to the nLC for separation of drug mixtures. Good separation was achieved for a methamphetamine and caffeine mixture, as well as for a morphine and cocaine mixture. These compounds were identified using the Viking National Institute of Standards and Technology (NIST) EI library. Application of this new technique to the separation and identification of novel psychoactive drugs, such as synthetic cathinones and synthetic cannabinoids, will be discussed. Once method development is completed, it is planned that the nLC/EI/MS will be tested in the field.

Reference(s):

1. P. Palma, G. Famiglini, H. Trufelli, E. Pierini, V. Termopoli, and A. Cappiello.Electron Ionization in LC-MS: Recent Developments and Applications of the Direct-EI LC-MS Interface. *Analytical and Bioanalytical Chemistry.* 399, (2011): 2683-2693, doi: 10.1007/s00216-010-4637-0.
2. A. Cappiello, G. Famiglini, E. Pierini, P. Palma, and H. Trufelli. Advanced Liquid Chromatography-Mass Spectrometry Interface Based on Electron Ionization. *Analytical Chemistry.* 79 (2007): 5364-5372.

Portable Nano-LC, LC/EI/MS, Drug Analysis