B56 Detection of Volatile Drugs of Abuse and Related Compounds in Breath Using Ion Mobility Spectrometry

Amy R. Aylor, BS, and Joshua A. Gunn, BFSc, West Virginia University, C. Eugene Bennett Department of Chemistry, 217 Clark Hall, Morgantown, WV 26506*

The goal of this presentation is to discuss the use of ion mobility spectrometry (IMS) to screen breath for the presence of volatile drugs of abuse and related compounds. Attendees will learn of the potential for IMS to be used for such an application and the supporting evidence and concepts for such a claim.

This presentation will impact the forensic community and/or humanity by proving the concept that volatile pyrolytic products of drugs of abuse may potentially be screened for using a method analogous to that used for blood-alcohol.

The analysis of breath as a screening tool for the estimation of blood alcohol concentration is a scientifically and legally validated technology. Because breath sampling is non-invasive, it represents an ideal forensic sampling matrix. Clinically, significant attention has been paid to the detection of volatile metabolites and biomarkers of lung cancer detected in exhaled air. Other studies have focused on exhaled breath as a means of assessing exposure to volatile organic compounds. However, aside from breath alcohol, few applications have been reported in the forensic arena.

Smoked drugs of abuse, such as methamphetamine, cocaine, and phencyclidine (PCP) enter alveolar gas during and immediately following inhalation. A portion of these is immediately exhaled, while another portion will adsorb into lung tissues. The remainder equilibrates rapidly with organic compounds in the capillary blood to enter the bloodstream. Following pulmonary output, metabolites again rapidly equilibrate with alveolar gas volatile compounds and comprise alveolar breath during the expiratory phase.

Breath is a plentiful sample matrix available for screening tests in forensic toxicology. Sampling is non-invasive and the general methodology has been vetted by over half a century of breath alcohol testing. The goal of the present study was to provide proof-of-concept for the use of ion mobility spectrometry (IMS) to screen breath for a larger pool of volatiles associated with drugs of abuse. Drugs of abuse and related compounds, such as pyrolitic products and the following known biomarkers of smoked methamphetamine, cocaine, and phenylcyclidine (PCP), respectively: 1-phenylpropene, anhydroecgonine methyl ester (AEME), and 1-phenyl-1-cyclohexene. Ethanol, methanol, isopropanol, acetaldehyde, acetone, caffeine, and nicotine were examined as possible interferents. Henry's law constants (K_H) and pharmacokinetic parameters were used to estimate the range of expected breath concentrations. IMS response in positive ion mode was determined across this range from aqueous solutions and air. Limits of detection for these compounds were found to be in the low parts-per-million range in breath for all compounds, corresponding to typical blood concentration levels reported in the literature. No significant interferences were noted.

Pyrolysis, IMS, Drugs of Abuse

 ** Presenting Author*