B113 Rapid Screening of Emerging Novel Psychoactive Substances (NPS) Using a Portable, Ambient Sampling Mass Spectrometer (MS)

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After attending this presentation, attendees will better understand how the merging of ambient ionization techniques and portable mass spectrometric technologies can be utilized to rapidly characterize new psychoactive substances onsite and offer high throughput detection via automated library searching methods of evidence ranging from trace residues surfaces to paraphernalia types, such as blotter paper.

This presentation will impact the forensic science community by introducing attendees to recent advances in portable, ambient sampling MS technology and the application of such a system for the analysis of new psychoactive substances.

The creation and use of NPS continues to increase throughout the world. In Europe alone, it has been reported that from the period of 2005-2014, over 400 NPS were reported to the European Union Early Warning System. In 2014, it was estimated that two NPS appeared on the market every week.[1] NPS are unregulated recreational drugs that have been synthetically modified to mimic traditional drugs of abuse while avoiding scheduling as an illicit substance. NPS pose a serious challenge for forensic identification in comparison to traditional drugs of abuse as structural characteristics can be variable and unknown.[2] The frequency and complexity of NPS evidence point to the need for robust screening methods, particularly portable technologies that could expedite legal investigations and reduce the burden on the crime laboratory system. In this study, a portable MS coupled with conventional and ambient ionization methods, such as Desorption Electrospray Ionization (DESI) and Paper Spray Ionization (PSI), was investigated as a flexible asset to combat the emerging threat of NPS.[3,4]

Substituted phenethylamines, particularly the 2C-series and prominent analogues featuring the addition of *N*-benzylmethoxy derivatives (i.e., NBOMes or "N-bombs") were the focus of this study. Analytical standards and mock forensic evidence were investigated via ESI, DESI, and PSI on a FLIR® Systems AI-MS 1.2 portable Cylindrical Ion Trap (CIT) MS.[5,6] The FLIR® Systems AI-MS 1.2, ruggedized for fieldwork, features an atmospheric capillary inlet with on-board high voltage and syringe pumping for coupling to conventional and ambient ionization methods. Both MS and Tandem Mass Spectrometry (MS/MS) data were collected for all analytes of interest in this study, incorporated into a simplified user interface that allows automated identification of threats via data dependent scanning and spectral database matching.[7] Automated spectral interpretation and simplified ionization methods, in turn, allow the collection of reliable and accurate data by non-technical users and first response personnel.

Data collected in this study suggest the use of interchangeable ionization sources outfitted on the AI-MS 1.2 system can provide a high throughput fieldable solution for NPS identification. Trace analysis, in the form of surface residues, was demonstrated by determining Limits of Detection (LODs) via surface swabbing PSI/MS from

a variety of surfaces of forensic relevance. LODs ranged from low to high nanograms of deposited analyte from the relatively smooth surfaces (i.e., glass, aluminum, plastic identification and electronic entry cards, and plastic storage bags) and textured and geometrically complex substrates (i.e., brass key, ceramic floor tile, and textured laminate countertop). Furthermore, application to realistic paraphernalia types, such as blotter paper, was shown, allowing accurate identification of illicit species even when present in complex mixtures.

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Field Analysis, Ambient Mass Spectrometry, NPS Detection