APPLICATION NOTE

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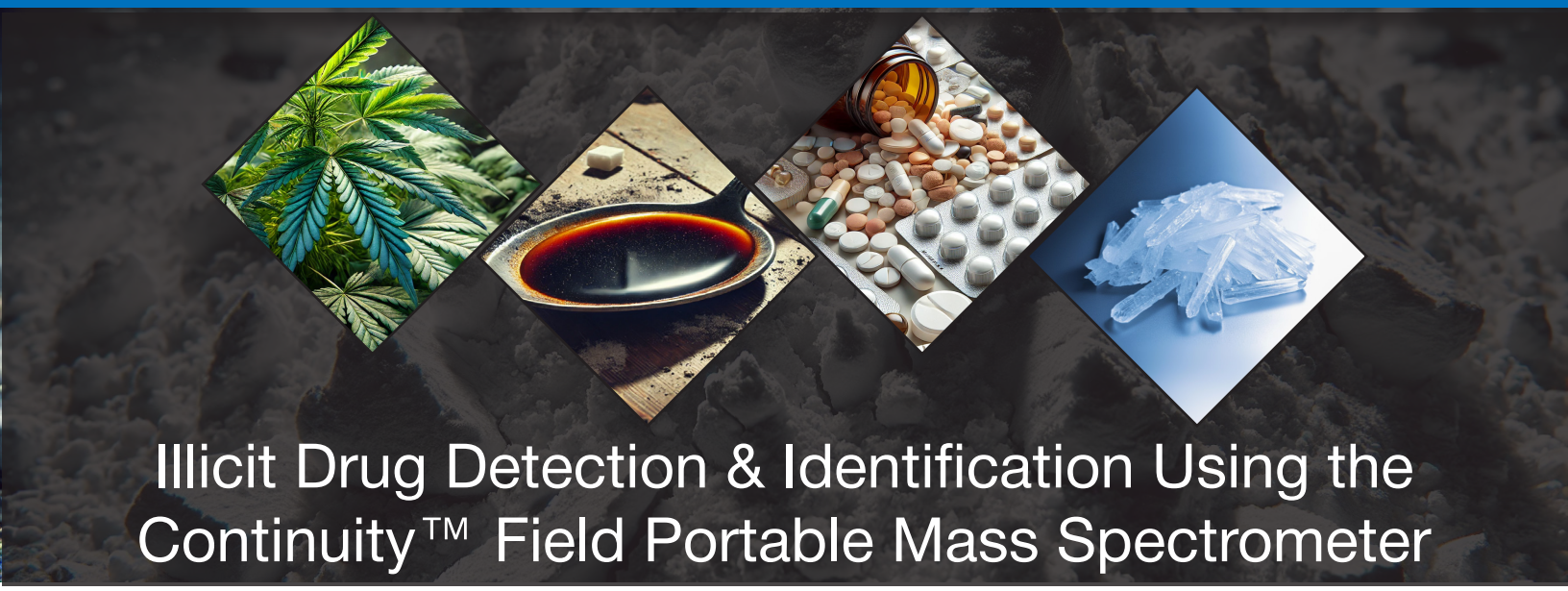

Illicit Drug Detection & Identification Using the Continuity™ Field Portable Mass Spectrometer

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Keywords

Portable MS, drugs, opioids, fentanyl, opiates, amphetamines

Objective

Detection, identification, and quantification of a series of drugs sampled from various surfaces.

Introduction

The trafficking and abuse of illicit drugs inflict tremendous harm upon individuals, families, and communities throughout the United States and the world. Based on the report of the United Nations Office on Drugs and Crime, nearly 296 million people worldwide used drugs in 2022, with an estimated 64 million suffering from drug use disorders. The opioid epidemic alone has claimed over 160,000 lives in the United States over the past two years, highlighting the urgent need for effective measures to combat this scourge.

Traditional methods of drug detection, such as laboratory-based analysis, are often time-consuming, costly, and require specialized personnel. These limitations make it challenging to address the rapid and widespread nature of drug trafficking and abuse. Moreover, the constant evolution of synthetic drugs and new psychoactive substances poses a significant challenge for law enforcement and public health officials, as these substances often evade detection using conventional methods.

In recent years, portable mass spectrometry has emerged as a promising solution for the rapid detection and identification of illicit drugs. Unlike traditional laboratory instruments, portable mass spectrometers offer the advantage of on-site analysis, enabling law enforcement officers and first responders to quickly identify substances in real-time. This technology can be deployed in various settings, including border checkpoints, public events, and field investigations, providing a versatile and efficient tool for combating drug-related crimes. As the opioid crisis and the rise of synthetic drugs continue to pose significant challenges, the integration of portable mass spectrometry into drug detection strategies represents a critical step towards a safer and healthier society.

Scenario and relevance

At border checkpoints, agents frequently encounter vehicles suspected of transporting illicit drugs. The ability to rapidly and accurately identify these substances is crucial for preventing trafficking and ensuring the security of the nation. Portable mass spectrometry offers an efficient solution for immediate, on-site analysis, enabling law enforcement to make informed decisions in real-time.

Figure 1. Security checkpoints can greatly benefit from the advanced capabilities of the Continuity™ Portable Mass Spectrometer.

The Continuity™ Field Portable Mass Spectrometer, equipped with a Swab-APCI (Atmospheric Pressure Chemical Ionization) source, can swiftly analyze trace amounts of illicit substances on various surfaces, including vehicle interiors, luggage, and clothing, without the need for extensive sample preparation. The process involves swabbing the suspected surface, inserting the swab into the Continuity™ system, and vaporizing the collected sample. The instrument then performs tandem mass spectrometry (MS^2) to identify the specific substances present. This capability allows border agents to efficiently screen for and identify illicit drugs on-site, thereby enhancing border security and preventing the entry of harmful substances.

Beyond border security, the application of this technology extends to airport security and other high-traffic areas where rapid drug detection is essential. TSA agents can utilize the Continuity™ system to swiftly screen passenger belongings for illicit drugs, contributing to safer travel environments. The ability to conduct these analyses on the spot significantly reduces the time and resources required for drug detection, making it a valuable tool for maintaining public safety.

Methamphetamine, cocaine, fentanyl, and MDMA are among the most prevalent and dangerous street drugs transported worldwide. In this application note, we showcase the robust analytical capabilities of the Continuity™ Field Portable Mass Spectrometer in detecting these compounds and other common illicit substances. Our study emphasizes the impressive limits of detection (LODs) of the instrument and its high sampling efficiencies across various surfaces, including glass, metal, and synthetic leather. This versatility underscores the Continuity™'s practical application in real-world scenarios, providing law enforcement and security personnel with a reliable and efficient tool for rapid on-site drug detection and identification. Moreover, the system's portability and ease of use make it an indispensable asset in the fight against drug trafficking and abuse, offering a crucial advantage in a wide range of operational settings.

Experimental

Standards and solutions

Standards were purchased from Cerilliant Corporation (Round Rock, TX, USA). Methanol (MeOH) of LC/MS grade was obtained from Sigma-Aldrich (St. Louis, MO, USA).

The commercial individual standard stock solutions were either 1 mg/mL or 100 µg/mL in MeOH or acetonitrile (ACN). All stock solutions were stored in a freezer at –20 °C. The 6-point calibration curves were prepared by serial dilution using MeOH, with concentrations in the range of 0.5 to 100 ng/µL.

Instrumentation

BaySpec Continuity™ Portable Mass Spectrometer was used equipped with a Swab-APCI source, specifically designed for TSA-approved swabs. The samples on swabs were converted into vapors *via* the Swab vaporizer unit, which then were drawn into the ionization chamber by the built-in sampling pump.

Measurements

The Swab-APCI source was operated at a constant temperature of 230 °C with a sampling gas flow rate of 800 mL/min. The APCI needle voltage was maintained at 3.5 kV throughout all experiments. The Continuity measurement software was run in full scan mode until an analyte's MS^1 peaks were detected, which then triggered the automated MS^2 experiments to isolate and fragment the precursor ions.

Calibration curves

The calibration curve standards were spotted onto TSA-approved Teflon®-coated fiberglass swabs from DSA Detection (North Andover, MA, USA). The solvent was allowed to evaporate before the swabs were introduced into the vaporizer.

Surface sampling

100 ng of the four selected analytes were spotted on the surfaces of individual glass, metal, and leather pieces and left to fully dry. TSA-approved Teflon®-coated fiberglass swabs from DSA Detection were used to sample each surface, and the recovery rate was calculated based on the calibration curves.

Figure 2. BaySpec Continuity™ Portable Mass Spectrometer equipped with a Swab-APCI source.

Results and discussion

A total of 10 drug standards were serially diluted in MeOH to create calibration curves and determine the Limit of Detection (LOD) of the Continuity™ portable MS equipped with the Swab-APCI ionization source. The measurements were run in triplicate, and the average value was used when creating the curves. LODs were determined as 5 times the baseline noise of the MS^2 experiments and are listed in Table 1 below. The calibration curves do not only provide a quantitative measure of the instrument's detection capability but also serve as a basis for calculating the swabbing efficiency from various surfaces.

Table 1. Limits of Detection (LOD) and the tracked MS^1 and MS^2 ions for all analytes.

Analyte	LOD (ng)	Precursor ion (*m/z*)	Fragment Ion (*m/z*)
Cocaine	0.47	304.2	182.0
Dexmedetomidine	1.22	201.1	95.1
Fentanyl	0.39	337.2	188.1
Heroin	2.30	370.2	165.1
Ketamine	3.11	238.1	125.1
MDMA	0.73	194.1	163.0
Methamphetamine	1.45	150.1	119.1
Norfentanyl	0.41	233.2	84.1
Oxycodone	0.84	316.2	298.1
Xylazine	0.63	221.1	164.1

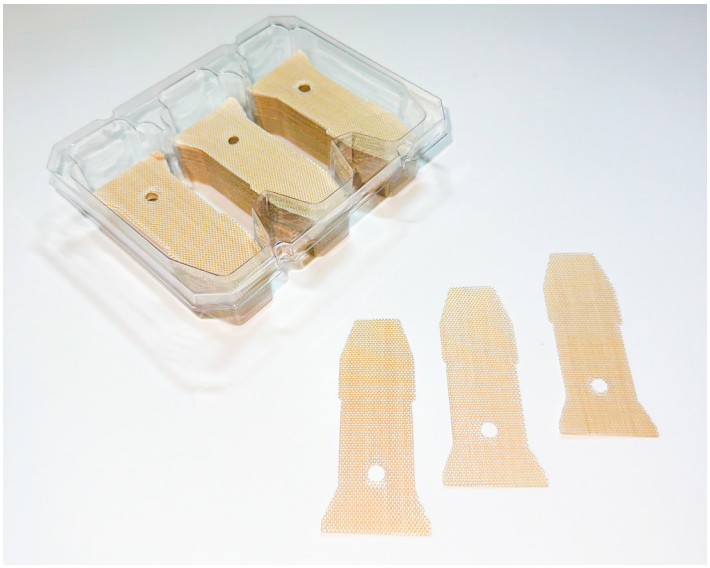

Figure 3. TSA-approved Teflon®-coated sampling swabs used in this study.

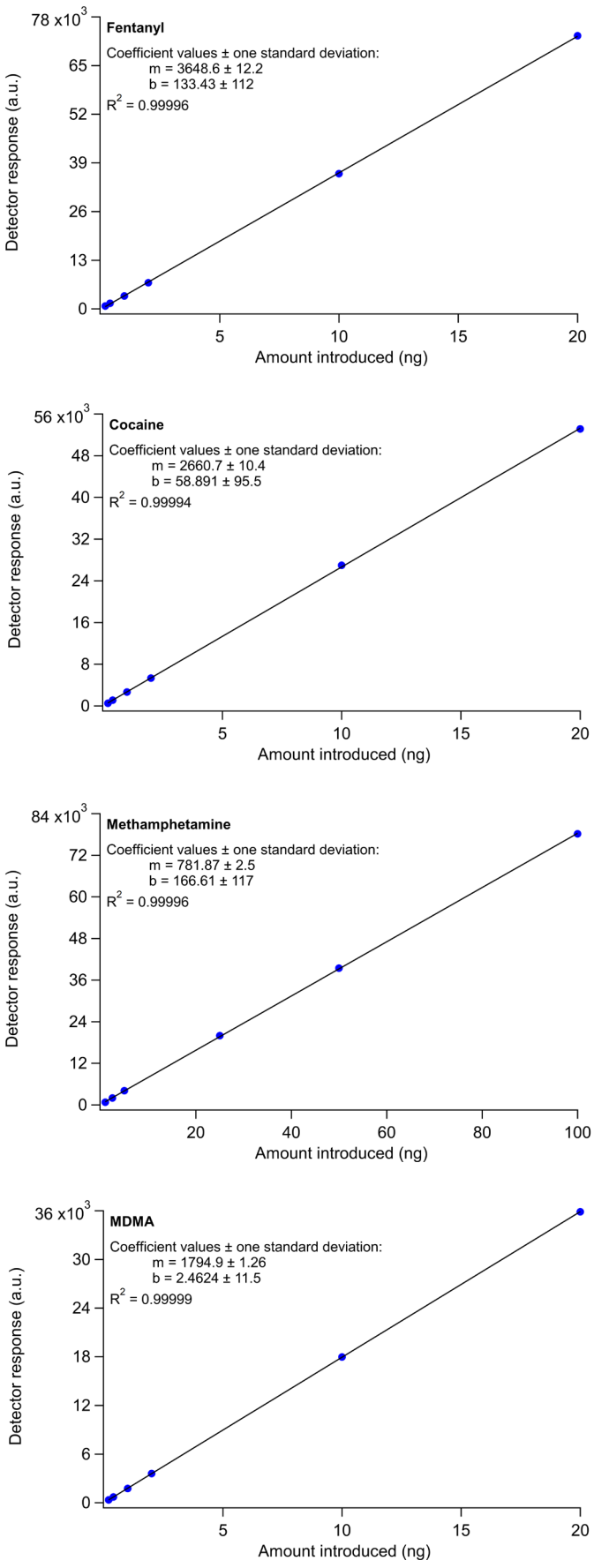

Figure 4. Calibration curves for select drugs used for LOD determination and for the recovery experiments.

For the surface sampling experiments, four analytes were selected: fentanyl, cocaine, methamphetamine, and MDMA. Three types of surfaces were chosen to represent different materials: glass, metal, and synthetic leather. For the glass, standard borosilicate microscope slides were used. The metal surface was represented by unpolished 6061 aluminum sheets, the most commonly used aluminum alloy, which were cut into pieces measuring 3 x 5 cm. Synthetic leather was selected over traditional cow leather due to its controlled surface roughness and environmentally friendly properties.

To ensure uniform distribution, the spotting of the analytes was performed using an analytical pipette. The sample was carefully pipetted on the surface, ensuring it spread only within a 1 cm diameter circle. After spotting, the solvent was allowed to completely evaporate, leaving behind an invisible dry residue. For sampling, a TSA-approved swab was used to collect the analyte from each surface. The swabbing process involved a consistent downward pressing motion combined with a left-to-right swipe, lasting approximately 5 seconds to cover the entire sample area.

Immediately after swabbing, the collected sample was introduced into the vaporizer of the Swab-APCI source for analysis. This rapid transfer helps to minimize any potential loss of the sample and ensures accurate detection. To determine the sampling efficiency, three replicates were performed for each analyte on each surface type. The data collected from these replicates were used to calculate the average sampling efficiency percentage for each analyte on the different surfaces.

These experiments aimed to assess the reliability and consistency of the Swab-APCI method across various common materials. The choice of surfaces reflects a range of real-world scenarios where illicit substances might be encountered, from smooth and reflective to rough and absorbent. The results of these experiments, including the sampling efficiencies and any observed variations, are presented in Figure 5 below. This data provides valuable insights into the effectiveness of the portable MS system in detecting and identifying trace amounts of drugs on different substrates.

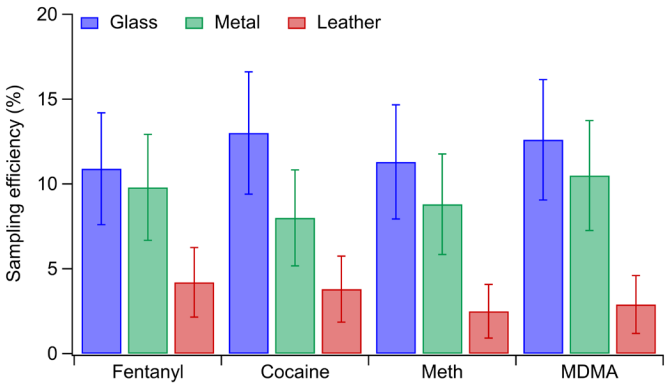

Figure 5. Recovery of fentanyl, cocaine, methamphetamine, and MDMA from glass, metal and leather surfaces.

Conclusions

In this study, we demonstrated the use of the Continuity™ Field Portable Mass Spectrometer equipped with a Swab-APCI ionization source for the detection and identification of various drugs. The capabilities of the instrument were assessed through the creation of calibration curves and surface sampling experiments using ten drug standards and four selected analytes: fentanyl, cocaine, methamphetamine, and MDMA. By serial diluting these standards in methanol, we established calibration curves and determined the instrument's Limits of Detection (LODs) in MS^2 mode. These experiments highlighted the instrument's ability to detect trace amounts of drugs with high sensitivity and specificity.

The performance of the Continuity™ field portable mass spectrometer in both controlled and real-world scenarios underscores its potential as a rapid, on-site analytical tool. The results obtained from triplicate measurements reinforce the reliability of this method, making it a valuable asset for law enforcement and public health agencies in their efforts to combat drug-related issues. This study confirms that the portable MS system can quickly and effectively identify illicit substances, offering a practical solution for field investigations and real-time decision-making. As the landscape of illicit drug use continues to evolve, such advancements in portable analytical technology will be crucial in providing timely and accurate information for intervention and prevention strategies.

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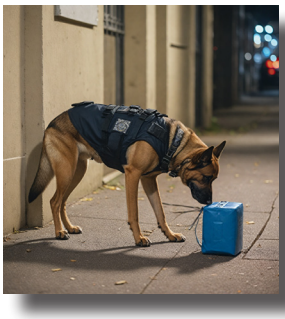



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