BAYSPEC

APPLICATION NOTE

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Field Explosives Detection with the Continuity™ Portable Mass Spectrometer

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Keywords

Portable MS, high explosives, low explosives, high energy materials

Objective

Detection, identification, and quantification of explosive compounds sampled from various surfaces in the field.

Introduction

The detection and prevention of explosive materials are paramount to ensuring public safety and national security, both within the United States and globally. The persistent threat of terrorist activities, coupled with the rise of homemade explosive devices, underscores the urgent need for advanced detection technologies. According to the Global Terrorism Database, over 8,000 terrorist attacks occurred worldwide in 2020, many involving improvised explosive devices (IEDs). The ability to detect and identify explosives before they are deployed is crucial in preventing such devastating events and protecting civilian lives.

Traditional methods for explosive detection, such as laboratory-based analysis and canine units, while effective, often face limitations due to high costs, logistical complexity, and the time required for thorough analysis. These challenges are especially pronounced in dynamic environments like transportation hubs, large public gatherings, and conflict zones, where the capacity to rapidly identify explosive materials can be the difference between life and death.

In recent years, portable mass spectrometry has emerged as a groundbreaking solution for the detection of explosive substances. Unlike conventional laboratory equipment, portable mass spectrometers facilitate real-time, on-site analysis, empowering security personnel, first responders, and military units to swiftly and accurately identify explosive compounds. This technology can be deployed in a variety of settings, from airports and border crossings to battlefield environments, offering a versatile and reliable tool for enhancing security measures. As the threat of terrorism continues to evolve, integrating portable mass spectrometry into explosive detection strategies represents a significant advancement in safeguarding communities and protecting critical infrastructure.

Scenario and relevance

Versatility in explosives detection

The Continuity™ Field Portable Mass Spectrometer, equipped with a Swab-APCI (Atmospheric Pressure Chemical Ionization) source, offers a powerful solution for rapid on-site detection of explosive materials. This system can quickly analyze trace amounts on surfaces such as vehicle interiors, luggage, and clothing without requiring extensive sample preparation. The process involves swabbing the surface, inserting the swab into the system, and vaporizing the sample, which is then subjected to tandem mass spectrometry (MS^2) to accurately identify specific explosive compounds. This versatility makes the Continuity™ system an essential tool in diverse security scenarios.

Transportation security and public safety

In environments like airports and transportation hubs, where the rapid detection of explosives is critical, the Continuity™ system proves invaluable. Its capability for immediate, on-site analysis enhances real-time screening processes, thereby improving public safety and reducing the risk of attacks. It could also be beneficial in subways, train stations, and other high-traffic areas, where rapid detection can prevent serious threats.

Applications in military and field operations

The portability and rapid analysis capabilities of the system make it particularly effective in military and conflict zones, where detecting improvised explosive devices (IEDs) is crucial. It can provide critical support to bomb disposal units and enhance situational awareness in the field. Furthermore, this technology is valuable in peacekeeping missions and humanitarian efforts, where the safe identification and removal of explosives are vital for protecting lives and maintaining stability.

Protecting critical infrastructure

The Continuity™ system also demonstrates significant potential in safeguarding critical infrastructure, including power plants, government buildings, and public landmarks. Its ability to detect a wide range of explosives across various surfaces makes it a robust and reliable tool for enhancing security in these sensitive and high-risk environments.

Figure 1. BaySpec Continuity™ Portable Mass Spectrometer equipped with a Swab-APCI source.

Experimental

Standards and solutions

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

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

Instrumentation

A BaySpec Continuity™ Portable Mass Spectrometer equipped with a Swab-APCI source was used in these experiments. The ionization source was specifically designed to accommodate TSA-approved swabs. The samples on swabs were vaporized in the Swab vaporizer unit and subsequently drawn into the ionization chamber by the built-in sampling pump.

Measurements

The Swab-APCI source was consistently maintained at a temperature of 250 °C, with a sampling gas flow rate set at 800 mL/min. Throughout all experiments, the APCI needle voltage was kept at $-3.0\ kV_{DC}$.

Calibration curves

Calibration standards were applied to 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 for analysis. The Continuity™ system was operated in full scan mode to monitor analyte MS^1 peaks. Upon detection of these peaks, the system automatically triggered MS^2 experiments, isolating and fragmenting the precursor ions to confirm the identity of the analytes.

Blast pit testing

To efficiently sample sand, adhesive sticky notes were utilized. The adhesive side of the note was able to collect a small amount of sand (less than 100 mg), which was then inserted directly into the vaporizer of the Swab-APCI source. During this testing, the Continuity™ system was operated in Target mode, performing direct MS^2 experiments by isolating and fragmenting the TNT MS^1 peak at *m/z* 226. The presence of TNT was confirmed by the appearance of the characteristic MS^2 peak at *m/z* 197. Target mode allows for rapid analysis without recording any MS^1 data.

Sensitive site testing

TSA-approved Teflon®-coated fiberglass swabs from DSA Detection were used to sample various surfaces during sensitive site testing. The Continuity™ system was again operated in Target mode, where direct MS^2 experiments were performed by isolating and fragmenting the RDX and HMX MS^1 peaks at *m/z* 284 and 358, respectively. The presence of these explosives was confirmed by the appearance of their respective MS^2 peaks at *m/z* 92 for RDX and *m/z* 147 for HMX.

Results and discussion

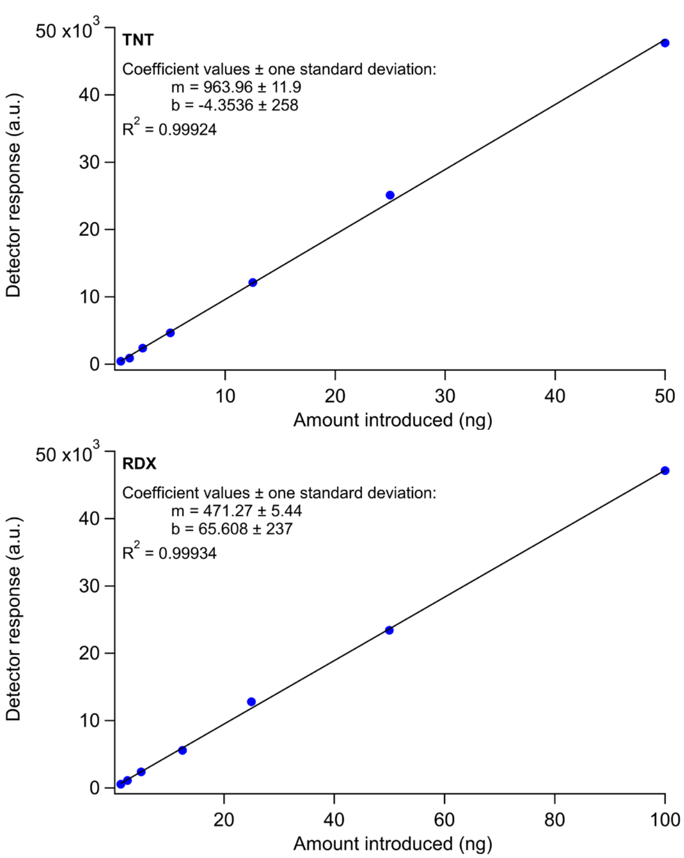
Calibration curves

Four explosive standards—TNT, RDX, HMX, and PETN—were serially diluted in methanol to create calibration curves and determine the Limit of Detection (LOD) using the Continuity™ portable MS equipped with the Swab-APCI ionization source. The LODs were calculated as five times the baseline noise of the MS^2 experiments and are presented in Table 1. These calibration curves not only provide a quantitative measure of the instrument's detection capability in a laboratory environment but also serve as a foundation for calculating the swabbing efficiency from various surfaces.

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

Analyte	LOD (ng)	Precursor ion (*m/z*)	Fragment Ion (*m/z*)
TNT	1.71	226.0	197.0
RDX	3.35	284.0	92.0
HMX	3.99	358.0	147.0
PETN	7.96	378.0	190.1

The calibration curves for the studied explosives exhibit a strong linear relationship between the amount introduced and the detector response, with R^2 values greater than 0.999. The limits of detection for all explosives are below 10 ng, indicating that the Continuity™ portable mass spectrometer's high sensitivity and reliability for quantitative analysis in trace-level explosive detection.



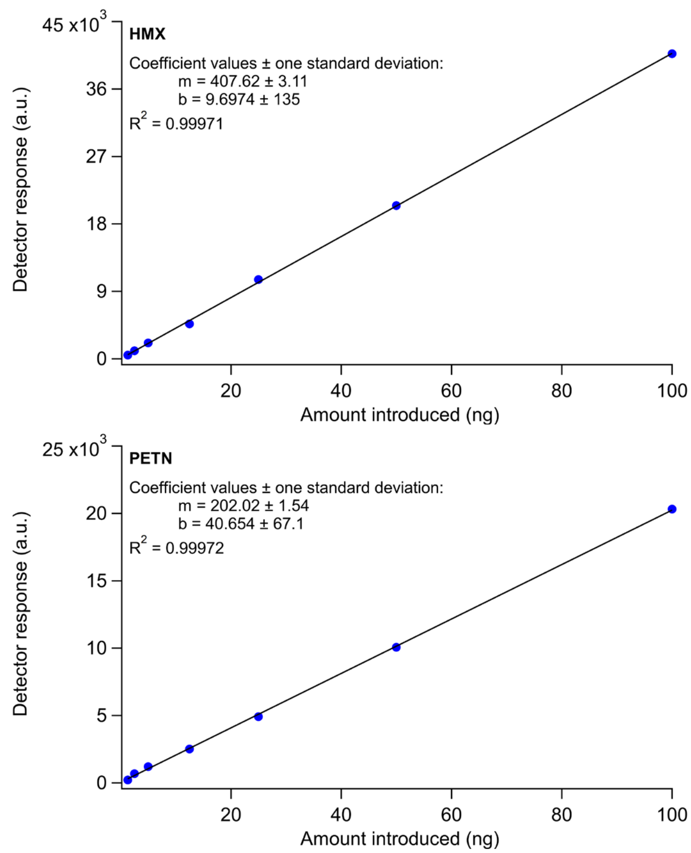


Figure 2. Calibration curves for TNT, RDX, HMX, and PETN used for LOD determination.

To validate the effectiveness of the Continuity™ Portable Mass Spectrometer in real-world scenarios, a series of field tests were conducted to demonstrate its analytical capabilities in detecting explosives. These applications underscore the instrument's potential not only in environmental monitoring but also in the identification of explosive materials, providing critical insights for weapons development and hazard mitigation.

Blast pit testing

At an authorized open-air detonation site in China Lake, CA, flake TNT explosives were detonated, leaving trace amounts of TNT and its nitroaromatic degradation products adsorbed onto nearby soil particles. To evaluate the residual presence of TNT, approximately 100 mg of sand was collected from two test blast pits using the adhesive side of standard office-use sticky notes. These sticky notes were then directly inserted into the Swab-APCI vaporizer for rapid and precise analysis. During the blast pit testing, only TNT detection was permitted. Therefore, the Continuity™ system was operated in Target mode, where direct MS^2 experiments were performed without recording any MS^1 spectra. This limitation was imposed to ensure that classified experimental explosives present at the site could not be inadvertently identified.

For Blast Pit #1, which had been inactive for 4 months, triplicate samples were collected at distances of 0, 3, and 6 meters from the center of the pit. For Blast Pit #2, inactive for 2 weeks, triplicate samples were taken from the center and 2 meters from the center of the pit. Additionally, samples were gathered from relevant surfaces, including the gloves and boots used during sampling, the tires of the vehicle used to reach the blast site, as well as the door handles of a nearby laboratory. As shown in Table 2, TNT was detected at all test locations except for the door handles of the nearby laboratory, confirming that safety protocols were adhered to and that the lab environment remained uncontaminated by TNT.

Table 2. Detection of TNT in sand and other surfaces near blast pits using sticky note sampling with Swab-APCI.

Location	Sample source	Sample number	Test result
Pit 1	Center	1	+
		2	+
		3	+
	3 m from center	1	+
		2	+
		3	+
	6 m from center	1	+
		2	+
		3	+
Pit 2	Center	1	+
		2	+
		3	+
	2 m from center	1	+
		2	+
		3	+
Other sufaces	Gloves		+
	Truck tires		+
	Boots		+
	Door handle (outside)		-
	Door handle (inside)		-

Figure 3. Rear view of the truck used to both approach the blast pits and to perform immediate analysis on the samples collected. The Continuity™ portable mass spectrometer is in the truck bed on the left partially covered by the operator and powered by an external battery on the right. A field operator is seen analyzing the collected samples on-site, demonstrating the capability of the instrument for immediate, in-field analysis. This simple setup highlights the portability and adaptability of the Continuity™ system for rapid deployment in remote and challenging environments.

Figure 4. Open blast pit of the Naval Air Weapons Station at China Lake used to safely dispose waste TNT and other high and low explosives.

Sensitive Site Testing

In the context of high-energy material production, real-time detection of explosives is critical to ensure a contamination-free environment. At the certified explosives mixing facility of the China Lake Naval Air Weapons Station, several surfaces were sampled using TSA-approved Teflon®-coated fiberglass swabs and analyzed with the Continuity™ mass spectrometer equipped with the Swab-APCI source, specifically designed for this swab. Due to the sensitive nature of the site, only HMX, and RDX were permitted to be detected. The Continuity™ system operated in Target mode, conducting direct MS^2 experiments without recording any MS^1 spectra, thereby preventing the inadvertent identification of classified experimental explosives.

As summarized in Table 3, HMX and RDX were detected on a variety of surfaces throughout the facility, including the floors, hoods, balances, and even door handles across multiple rooms. Notably, HMX was detected in both the “dirty” hood of the shipping and receiving room, and on various surfaces within the explosives mixing room. The control room also revealed the presence of both HMX and RDX on surfaces, emphasizing the widespread nature of explosive residue in such an environment.

Table 3. Detection of HMX and RDX at an explosive mixing facility using Swab-APCI.

Location	Sample source	Detected explosives
Shipping & receiving room	“Clean” hood	–
	“Dirty” hood	HMX
	Floor	HMX
Explosives mixing room	Balances	HMX
	Floor	HMX
	Sink	HMX
	Mixer	HMX
Control room	Static tester for shoes	HMX, RDX
	Table	HMX, RDX
Laboratory	Lab hood, inside	HMX, RDX
	Lab hood, glass	–
	Door handle	HMX, RDX

These findings underscore the instrument's ability to rapidly and accurately identify explosives in a manufacturing environment, ensuring critical safety and contamination control measures are maintained.

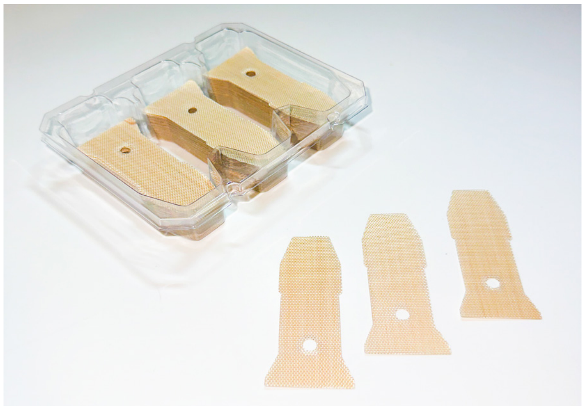


Figure 5. TSA-approved Teflon®-coated sampling swabs used to collect from the surfaces of the explosive mixing facility.

Conclusions

This study has demonstrated the exceptional capabilities of the Continuity™ Field Portable Mass Spectrometer, equipped with a Swab-APCI ionization source, in the detection and identification of explosive materials across a range of environments. Calibration curves for TNT, RDX, HMX, and PETN provided a robust quantitative assessment, confirming the ability of the system to achieve low Limits of Detection (LODs) with unparalleled sensitivity and accuracy in MS^2 mode. These results underscore the instrument's capacity to reliably identify trace levels of explosive compounds, critical in both laboratory and field settings.

The field applications conducted, including blast pit testing and sensitive site analysis at a certified explosives mixing facility, further validated the instrument's real-world utility. The Continuity™ system successfully detected residual explosives in complex environments, proving its robustness and reliability. The detection of HMX and RDX on a variety of surfaces, even in the presence of potential interferences, emphasizes the system's precision and effectiveness in ensuring environmental safety and contamination control.

These findings highlight the Continuity™ Portable Mass Spectrometer as an indispensable tool for security personnel, military operations, and industrial safety. Its rapid, on-site detection capabilities, combined with high sensitivity and accuracy, offer a significant advancement in the field of explosives detection. As global security challenges continue to evolve, the integration of such portable mass spectrometry technology into field operations can substantially enhance the ability to detect, mitigate, and respond to explosive threats, thereby contributing to the safety and security of both public and sensitive environments. The Continuity™ system not only meets but exceeds the rigorous demands of real-time explosives analysis, positioning it as a leading solution for ensuring public safety and national security in an increasingly complex threat landscape.

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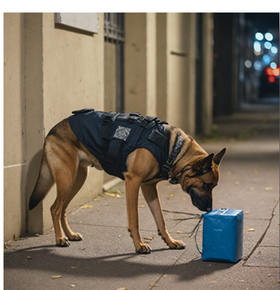



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