Evaluating the Suppression Tolerance of a Novel Walk-up Desktop Trace Detector

mass spec™
EXPERT TRACE DETECTION

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INTRODUCTION

Mass Spectrometry Trace Detection (MS-TD) has traditionally excelled in forensic labs, providing high-throughput analysis of trace surface samples. Mass Spec Analytical Ltd. (MSA) introduces a groundbreaking system, "NXT-Detect," that seeks to redefine desktop trace detection with swab sampling. The system identifies diverse threats (explosives, pesticides, drugs, chemical warfare simulants) using a novel approach.

Direct thermal analysis yields low nanogram range detection limits, while swabbed liquid samples dried on glass slides achieve sensitivities as low as 100ng. However, common interferents (cleaning products, cosmetics, oils) pose challenges, leading to false positives/negatives, excessive background noise, or inhibition.

Our poster addresses this issue by evaluating the prototype's suppression tolerance to everyday interferents. We explore how the system handles these challenges, paving the way for real-world deployments in accessible, walk-up systems. This research enhances mass spectrometry trace detection's applicability and reliability in threat detection and forensic analysis.

METHODS AND MATERIALS

Prototype System Overview:
This study employs a high-throughput prototype system for diverse threat trace analysis, integrating components from Mass Spec Analytical Ltd. (MSA) and Waters Instruments™. The system seamlessly combines the MSA Thermal Desorber (TD) Ion Source and the Waters RADIAN™ Single-Quad Mass Spectrometer (MS), showcasing advanced trace detection technology.

MSA TD Ion Source:
- MSA TD Source at 200˚ C, 9 L/min flow rate.
- Full Scan mode, 30-500 m/z range in negative polarity.
- 4-function method with optimized cone voltages.
- PTFE-coated fiberglass swabs used for Thermal Desorption.

Waters RADIAN™ Single-Quad MS:
- Robust mass analysis with variable cone voltage for tailored fragmentation.
- Swab analysis conducted using Waters MassLynx™ software.

Figure 1: MSA Prototype Thermal Desorber fitted to Waters RADIAN Instrument / PTFE-coated fiberglass swabs used for sample acquisition.

Explosive Compound Analysis:
Three diverse explosives selected – PETN, RDX, TNT – simultaneously detected in negative APCI mode.

Environment Sampling Methodology:
Environmental swabs from 30 locations, each swab inserted for 10 seconds with a 90-second interval between samples for baseline return. The check swabs act as reference points for performance assessment over time.

Interferant/Suppressant Analysis:
Eight common compounds known to affect detection techniques were selected including WD40 lubricant, hand sanitiser, cologne, three different multi-purpose cleaners and body moisturizer.

RESULTS

Environmental Tests

To assess the prototype's ability to handle background contaminants, over 500 environmental swabs were collected from a diverse range of locations, including homes, offices, vehicles, and public spaces.

Each swab was analysed following a rigorous protocol:
- 10-second insertion: Samples were introduced for a brief period to minimize background contamination.
- 90-second interval: Sufficient time was allowed for signal baseline recovery between samples.
- Check swabs: Clean swabs spiked with known explosives were analysed at regular intervals as a performance benchmark.

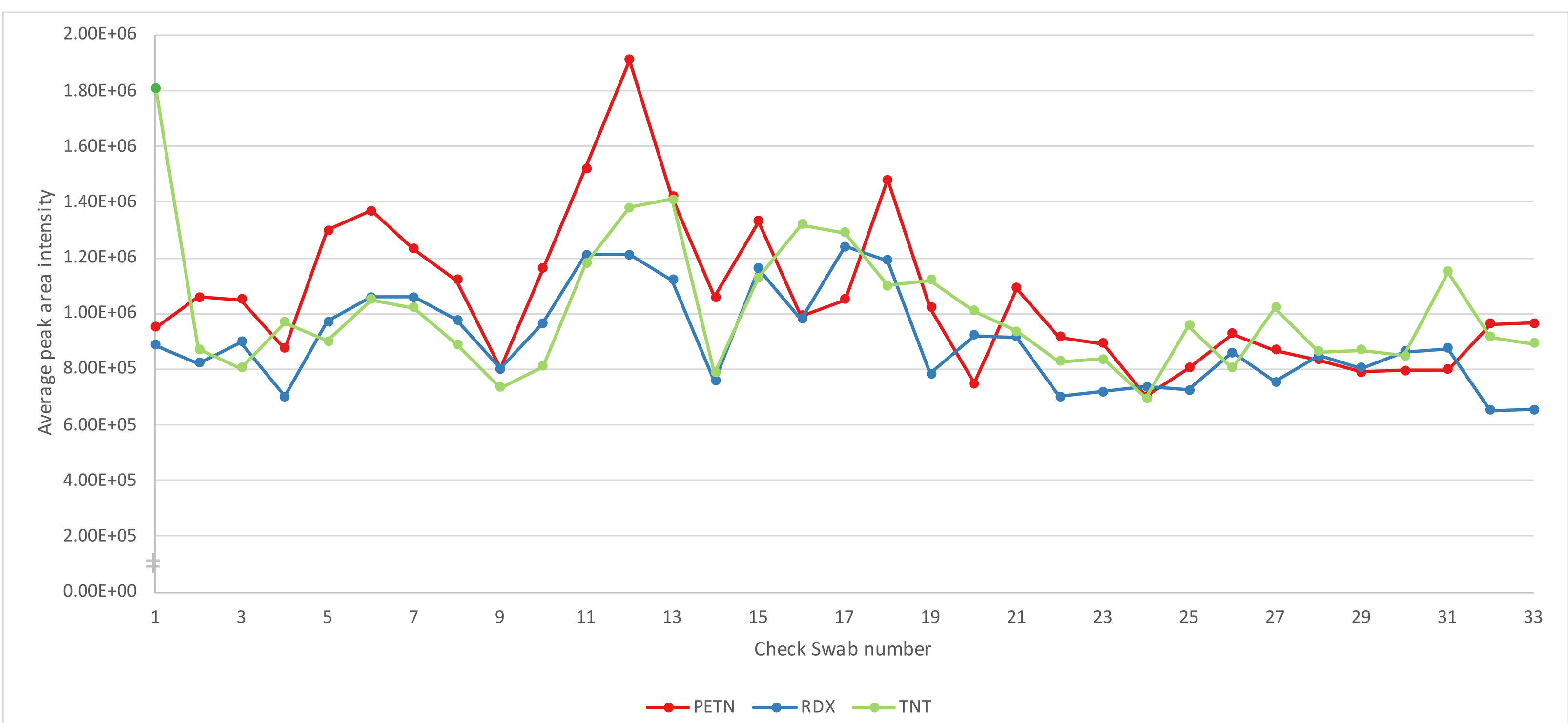


Figure 2. Peak areas for PETN, RDX, and TNT show a minor decline over environmental swabs, yet remain well within acceptable detection limits.

Over 447 analyses were conducted over a 7-hour period, with check swabs interspersed throughout. The results were encouraging:
- Minimal performance degradation: Check swabs consistently maintained acceptable detection levels, demonstrating the prototype's resilience to environmental contaminants.
- Gradual decline: The slow decrease in sensitivity over time allows for convenient monitoring and proactive intervention.

Extrinsic Residue Suppression

To assess the prototype's resilience to common environmental interferents, known to hinder some detection techniques, eight readily encountered compounds were chosen, spanning colognes, cleaners, moisturizers, and hand sanitiser.

- Residues were applied to glass slides (3 per compound).
- RDX check swabs (100 ng) were analyzed following the established protocol.
- Residue acquisition involved a blank swab followed by three residue slide transfers.
- Samples were run in a specific order with interspersed check acquisitions.
- This process was repeated for PETN and TNT.

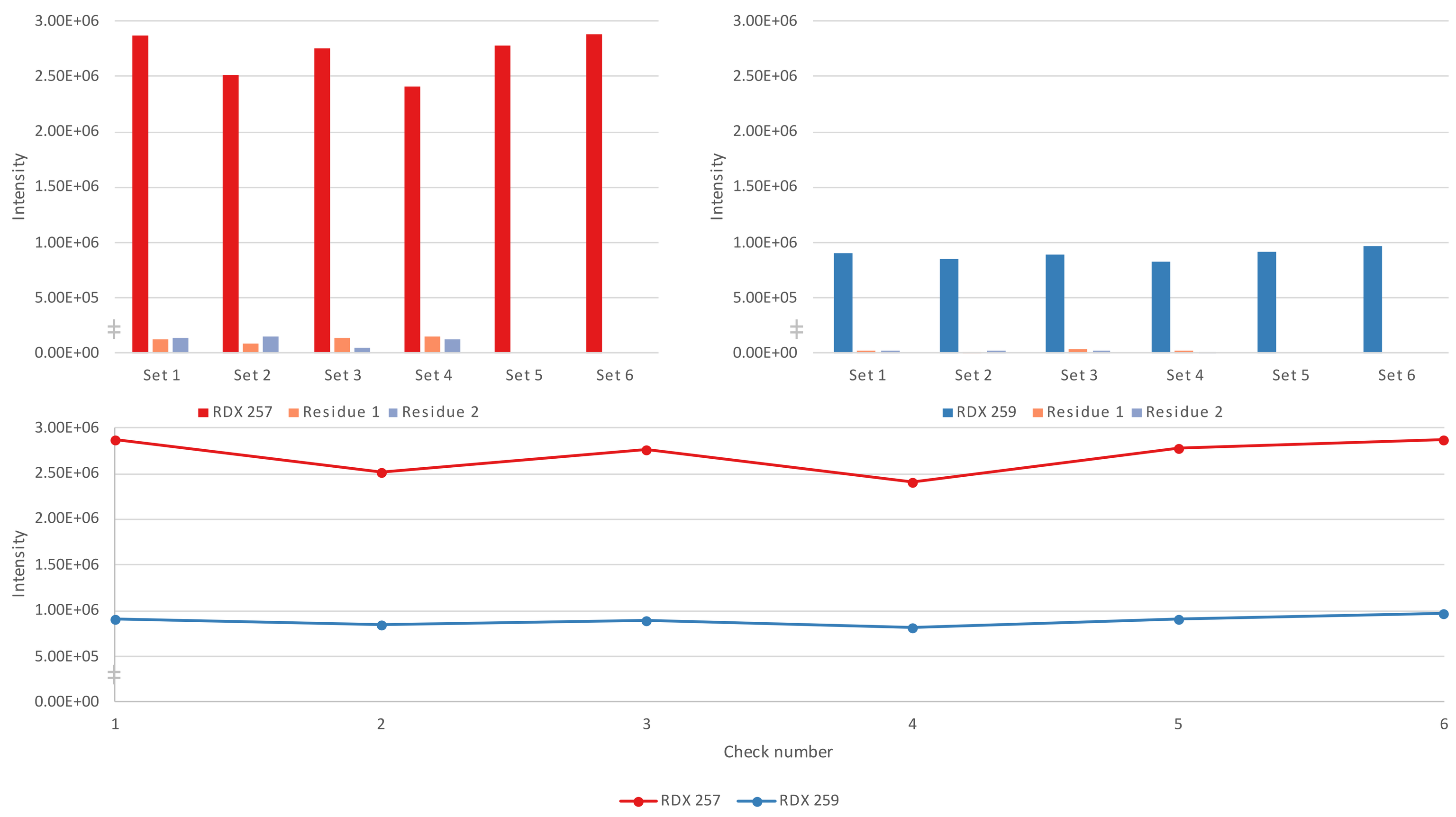


Figure 3: Top - RDX signal (257/259 m/z) dominates over residue background. Bottom - Individual m/z responses over the analysis, highlighting minimal impact of residues.

Figure 3 shows that the selected explosive signals significantly exceed the background noise induced by any residue (lower graphs). The graphs for PETN and TNT were very similar.

No noticeable performance decline was observed for any explosive check swabs throughout the investigation, despite analysing 24 residue samples per experiment.

Intrinsic Residue Suppression

This section explores the prototype's susceptibility to "intrinsic suppression," where interferents directly suppress the target explosive by competing for ions or raising background noise.

- Five residues from the previous experiment were chosen for individual and combined testing with each explosive.
- Residues were applied to glass slides, and combined swabs were prepared by transferring residue followed by spiking with 100ng of explosive.
- Three acquisitions were run for each combination: isolated explosive, residue only, and combined residue/explosive.
- This was repeated for RDX, PETN, and TNT (using furniture polish instead of multi-surface cleaner for PETN and TNT).

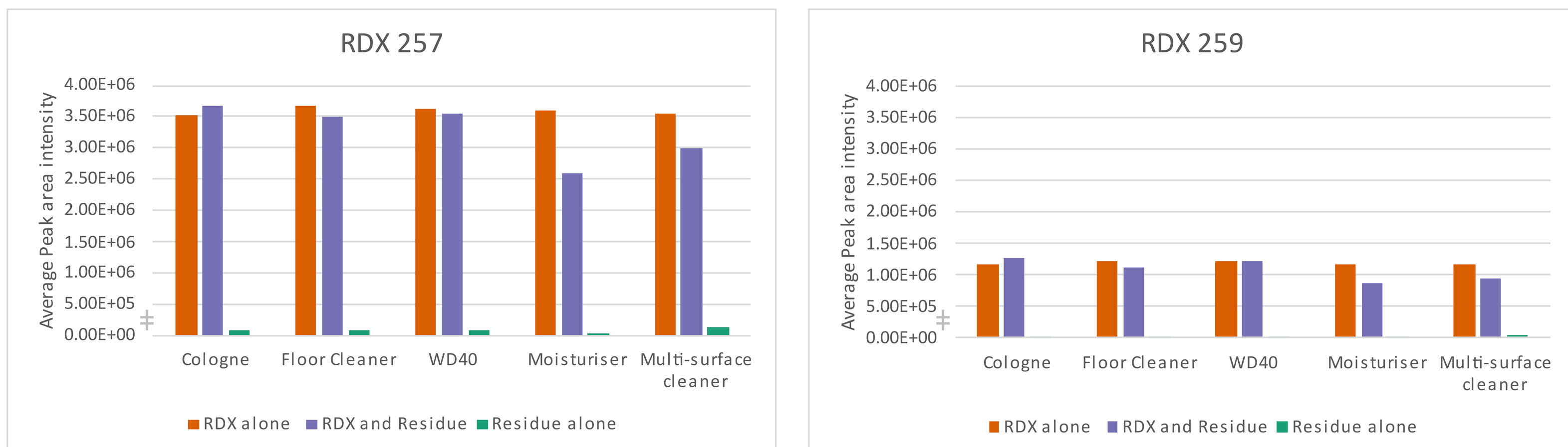
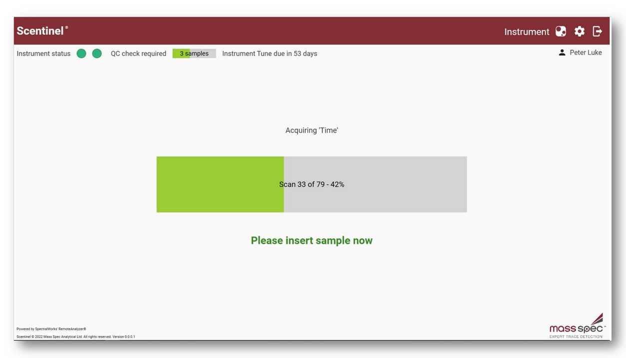


Figure 4: Responses of RDX 257/259 during intrinsic suppression investigation (no bar indicates there was no significant response after peak integration)

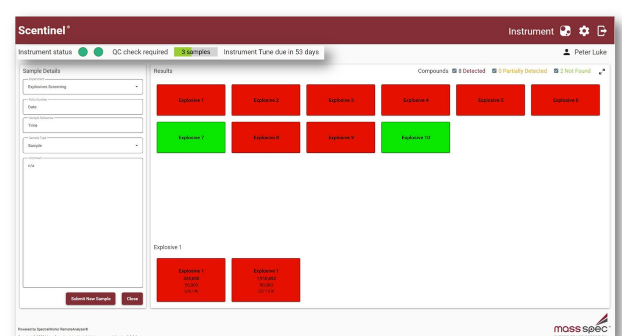
Figure 4 confirms intrinsic suppression, but the effect is not debilitating. Results for PETN and TNT are similar. TNT is most affected, likely due to its interaction with the chlorine used to analyze RDX and PETN. Moisturizer emerges as the most potent suppressor across all explosives due to its thick composition. Notably, the isolated explosive results suggest minimal extrinsic suppression from the residue sequence, implying the major impact comes from the combined swab.

REAL-WORLD APPLICATION

As a real-world application, consider the integration of this detector with MSA's Scentinel™ II Walk-up software for explosives detection, coupled with Spectralworks RemoteAnalyzer® for data analysis. This combination streamlines complex mass spectrometry data into intuitive Yes/No results, empowering non-expert users like security personnel. A user-friendly touch-screen interface provides easy instrument operation, while instant feedback allows for immediate action.



Sample is acquired and results displayed.



1) **Collect sample.**
2) **Start analysis:** Use touchscreen or mouse to select sample type and method, then follow on-screen/audio prompts for swab insertion.
3) **View results:** Analysis takes 8-10 seconds. Screen displays compounds tested; positive results indicated in red.
4) **Review data:** Remote expert review via data archiving ensures trend analysis and future research capability.

This approach can be extended to other analytes of interest and has been demonstrated with drugs of abuse and pesticides.

CONCLUSIONS

Trials confirmed the prototype's exceptional environmental tolerance for reliable detection in harsh settings. Rapid analysis and proactive monitoring bolster field-ready potential. Minimal intrinsic suppression poses negligible real-world impact. This high-performance system, with its walk-up software, excels in diverse trace detection, especially under demanding conditions.