Open port sampling interface mass spectrometry of wipe-based explosives, oxidizers, and narcotics for trace contraband detection

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**Keywords**: Trace detection; Open port sampling interface; Mass spectrometry; Explosives; Narcotics

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**Abstract**

Rapid screening for chemical traces of explosives and narcotics is widely used to support homeland security and law enforcement. These target compounds span a range of physicochemical properties from organic to inorganic, with preferential ionization pathways in both negative and positive mode operation. Nonvolatile inorganic oxidizers present in homemade fuel-oxidizer mixtures, pyrotechnics, and propellants create a unique challenge to traditional thermal desorption-based technologies. Developments in solid-liquid extraction techniques, specifically, open port sampling interface mass spectrometry (OPSI-MS) provide compelling capabilities to address these hurdles. In this proof of concept study, we investigated the trace detection of wipe-based (*i.e.,* common swipe sampling collection method) explosives, oxidizers, and narcotics using an OPSI source and compact single quadrupole mass analyzer. The liquid dissolution and extraction capabilities of OPSI enabled detection of both traditional military-grade explosives and homemade explosive oxidizers. OPSI-MS sensitivities to a series of seven target compounds from polytetrafluoroethylene (PTFE) coated fiberglass sampling wipes were on the order of several nanograms to sub-nanogram levels. Comparisons with direct solution-based sample analysis enabled quantification of wipe-based sample extraction effects. The system demonstrated quick temporal responses, polarity switching capabilities, and rapid signal decay with minimal carryover, all critical to high throughput screening applications. Coupling traditional swipe sampling with OPSI-MS offers a promising tool for contraband screening applications.

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**Introduction**

Analytical techniques capable of the rapid identification of trace particle residues from explosives and illegal narcotics (*i.e.,* trace contraband) are deployed worldwide to support aviation, mass transit, and customs screening checkpoints.1-3 Such high throughput screening technologies are also used to protect critical infrastructure and select public venues. Successful identification of trace contraband presumes that people or objects used for the transport or manufacture of explosives or illegal narcotics will be contaminated by trace particle residues in sufficient quantities to be detected by the screening technology employed.4, 5 A positive alarm may result in denial of entry through a security checkpoint or prompt additional law enforcement intervention. The utility of analytical techniques for trace screening is often driven by the specific concept of operations for a given user (*e.g.,* environment, size and portability constraints, throughput required) and the nature of the material targeted for detection (*e.g.,* drugs vs explosives, type of explosive). Regardless of specific operational considerations, common requirements for a trace screening instrument include low cost, field portability, short analysis times, high sensitivity, and selectivity for a range of threats and simple operation appropriate for relatively untrained end users.

While many analytical techniques have been applied to the trace screening arena, ion mobility spectrometry (IMS) has been the most widely deployed, particularly for aviation security, and meets the requirements listed above.6-8 IMS is based on measurement of the gas phase mobilities of unknown ions in a weak electric field at ambient pressure with identification by matching to reference mobility values of known contraband materials.9 Collection of contraband particles is generally achieved by swipe sampling of suspect surfaces followed by heating of the wipe to ≈230 °C (*i.e.,* thermal desorption) to convert solid particles into vapor for subsequent ionization and mobility analysis. While IMS finds extensive use in screening for common explosives and narcotics, the low vapor pressure of refractory inorganic oxidizer materials, common to homemade fuel-oxidizer explosives, remains problematic for thermal desorption-based sampling.10 These homemade explosives are generally based on readily available fuels (*e.g.,* sugar, petroleum jelly, or aluminum) and oxidizers (*e.g.,* potassium perchlorate or potassium nitrate) or already processed propellants and pyrotechnics. Such charges frequently top the annual U.S. Bomb Data Center Explosives Incident Report.11 Screening of common inorganic oxidizers often requires modifications for higher desorption temperatures12 or the use of specially modified chemical wipes for analysis.13, 14 A recent review focused on the unique challenges screening technologies face for trace detection of inorganic-based explosives, providing perspective and recent developments addressing these challenges.15 One of the main categories highlighted for addressing the nonvolatility of inorganic oxidizers was physical dissolution into an appropriate liquid. Techniques employing this avenue include, capillary electrophoresis,16-18 ion selective electrodes,19 and flow-injection analysis (FIA)20 or solid-liquid extraction ambient ionization platforms for mass spectrometry (MS).21-24

Solid-liquid extraction techniques are especially relevant to addressing some existing limitations by eliminating the need for thermal desorption to produce gas phase analyte molecules, extending the list of accessible and extractable analytes. These methods are often coupled with MS for mass analysis and identification. In general, IMS suffers from low(er) resolving power, making detection specificity of trace materials in complex chemical backgrounds challenging. Mass spectrometry enables advantages over IMS for screening applications by providing improved dynamic range, sensitivity, and selectivity.25 Due to these inherent benefits, MS-based trace detection has received considerable attention in recent years.26 This interest has coincided with the reduction in instrument size and advent of ambient ionization approaches such as direct analysis in real time (DART)27 and desorption electrospray ionization (DESI),28 among many others.29 Discussion of the advantages and limitations of various ambient ionization and related techniques for trace explosives detection may be found in a recent review.30

Developments in solid-liquid extraction approaches for direct liquid sampling of surfaces combined with MS for explosives and narcotics detection have been described in a number of publications.21-24, 31 The self-aspirating continuous flow open port sampling interface (OPSI) coupled with MS, as described by Van Berkel *et al.*,32, 33 is of specific interest to the current study. In this technique, coaxial tubes are used to provide both solvent flow to the OPSI interface via the annulus between the inner and outer concentric tubes and aspiration of solvent via the central tube into an electrospray ionization source (ESI) coupled to a mass spectrometer. The inlet flow rate of solvent is controlled by a syringe pump while the aspiration rate from the drop is controlled by the Venturi effect pulling solvent into the ESI-MS. Depending on the balance of input and output flows, several operational modes have been characterized, including, supercritical vortex, critical vortex, subcritical vortex, balanced, and convex spill over.34 Numerous modes of operation have been employed for surface scanning, semi-remote sampling, and aerosol or droplet collection. Various open port sampling interfaces and related techniques have found utility in a wide range of applications.31, 35-40

In this proof of concept study, we employ OPSI-MS in the “spill over” mode for trace screening of wipe-based organic explosives, inorganic oxidizers, and a narcotic. In this operational mode, the delivery rate of solvent exceeded the aspiration rate, creating a convex meniscus or hemispherical solvent dome at the source tip. Sampling wipes (*i.e.,* a polytetrafluoroethylene (PTFE)-coated fiberglass weave or *meta*-aramid substrates) directly touched the protruding solvent dome allowing for rapid extraction and transport of the analyte to ESI-MS for analysis. A compact single quadrupole mass analyzer was used to demonstrate a more fieldable instrument. We investigated system response and sensitivity for the analysis of wipe-based and direct solution introduced explosives, oxidizers, and narcotics. In addition, we characterized the repeatability and temporal response of the system, wipe material effects, polarity switching capabilities, and mixture analysis.

**Experimental Methods**

**Sample Preparation.** Samples were prepared by inkjet deposition with a JetLab 4XLb inkjet printer (Microfab Inc, Plano, TX) onto PTFE-coated fiberglass weave sampling wipes (DSA Detection, North Andover, MA, USA) and Nomex *meta-*aramid wipes (Smiths Detection, Edgewood, MD, USA). Detailed inkjet printing procedures are described elsewhere in the literature.41-43 Briefly, cocaine was printed using 1 mg/ml standard solution in acetonitrile (Cerilliant Corporation, Round Rock, TX, USA). 1,3,5-Trinitroperhydro-1,3,5-triazine (RDX), pentaerythritol tetranitrate (PETN), and trinitrotoluene (TNT) printing solutions were prepared from pure powders (Cerilliant Corporation) gravimetrically dissolved in 2-propanol (Fisher, HPLC Grade 2). Aqueous analytical standards of sodium nitrate (NaNO3), potassium chlorate (KClO3), and potassium perchlorate (KClO4) were purchased from Inorganic Ventures (Christiansburg, VA, USA). Samples were inkjet printed as single spots, yielding deposits with effective diameters on the order of 10’s of micrometers to 100’s of micrometers depending on mass.44 Mixture analysis was completed on Jim Shockey’s Gold, a black powder substitute propellant (provided by the Bureau of Alcohol, Tobacco, Firearms, and Explosives forensic laboratory). Jim Shockey’s Gold is a mixture of potassium perchlorate, potassium nitrate, and ascorbic acid.

Certain commercial equipment, instruments, or materials are identified in this article in order to specify the experimental procedure adequately. Such identification is not intended to imply recommendation or endorsement by NIST, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.

**OPSI-MS Analysis.** All experiments were performed on an expression single quadrupole mass spectrometer (Advion, Inc., Ithaca, NY, USA) coupled with a Touch Express open port sampling interface and electrospray ion source. The carrier solvent was 10 mmol/L ammonium acetate in a mix of acetonitrile and water (95/5, v/v) for organic compounds, and 10 mmol/L ammonium acetate in a mix of acetonitrile and water (50/50, v/v) for inorganic compounds. The solvent was delivered by an isocratic pump with a flow rate of 250 µL/min. The ion source settings for all target compounds were optimized by analyzing solution-based standards (1 µL of a 100 ng/µL standard solution) directly pipetted into the OPSI drop. The positive ESI settings included a 250 °C capillary temperature, +150 V capillary voltage, +20 V source voltage offset, 0 V source voltage span, 350 °C source gas temperature, and +4500 V ESI voltage. Optimal negative ESI settings were 150 °C capillary temperature, -150 V capillary voltage, 20 V source voltage offset, 0 V source voltage span, 350 °C source gas temperature, and -3500 V ESI voltage. The source gas was set to a flow rate of 3 L/min. The N2 gas pressure supplied to the OPSI was set to 552 kPa (nominally 80 psi) when using high organic solvent and 689 kPa (nominally 100 psi) for organic solvent/water mixtures. The scan mode, with a mass range from mass/charge (*m/z*)50 to *m/z* 500, and the selected ion monitoring (SIM) mode, with target *m/z* ratio, were used in each analysis.

**Results and Discussion**

**Observed Response and Sensitivities**

The OPSI-MS system was investigated for the analysis of wipe-based samples as shown schematically in Figures 1A and 1B. The system performance metrics, including representative mass spectra, response curves, and sensitivities, were measured for three organic explosives (RDX, TNT, and PETN), three inorganic oxidizers (KClO3, KClO4, and NaNO3), and a narcotic (cocaine). Characteristic base peak ions observed for each of the target analytes are listed in Table 1. Ion distributions for these compounds were consistent with similar ESI-MS analysis and as expected given solvent compositions. Figures 1C and 1D display representative full scan mass spectra for PETN and potassium perchlorate (remaining full scan mass spectra can be found in supporting information, Figure S1). The ammonium acetate component of the OPSI solvent yielded acetate (CH3COO-, abbreviated: OAc-) adduct formation with PETN (*m/z* 375 [PETN+OAc]-) and RDX (*m/z* 281 [RDX+OAc]-), as the dominant ions (Figures 1C and S1). The nitroaromatic TNT predominantly produced the deprotonated molecule (*m/z* 226 [TNT-H]-) in negative mode. Similarly, the narcotic cocaine produced the protonated molecule (*m/z* 304 [cocaine+H]+) and a common fragment (*m/z* 182) in positive mode. Finally, each of the inorganic salt ion distributions from full scan mass spectra were dominated by the bare anion (*i.e., m/z* 62 NO3-, *m/z* 83 ClO3-, and *m/z* 99 ClO4-). In addition to peaks generated by the analytes of interest, the OPSI solvent composition (ammonium acetate, acetonitrile [abbreviated: MeCN], and water) also led to minor ion and clusters, including, *m/z* 59 OAc-, *m/z* 119 (HOAc)(OAc)-, *m/z* 136 (NH4OAc)(OAc)-, and *m/z* 141 (MeCN)2(OAc)- (Figures 1C, 1D, and S1).



**Figure 1**. (A) Schematic representation of the OPSI-MS configuration and wipe-based sample introduction with (B) section A-A details (OPSI image provided by and reproduced with permission from Advion). Representative mass spectra for (C) PETN and (D) potassium perchlorate samples analyzed from PTFE-coated fiberglass weave wipes. Response curves for (E) PETN and (F) potassium perchlorate as a function of mass for both wipe-based samples and direct solution introduction to the OPSI solvent meniscus. Data points and uncertainty represent the average and standard deviation of replicate measurements (n=10 for wipe samples and n=5 for solution samples).

The OPSI-MS system response curves were measured for each analyte using PTFE-coated fiberglass weave wipes loaded with 1 ng, 10 ng, 30 ng, 100 ng, 300 ng, and 1000 ng depositions. Ten replicates were run for each mass loading of the wipe-based samples and peak areas extracted from selected ion monitoring of the dominant ion (Figures 1E, 1F, and S2). For each sample, the rough location of the wipe-based analyte deposit was brought into contact with the OPSI solvent meniscus (≈ 4 mm diameter) for 2 s to 3 s and slowly moved around the central region (± 2 mm to 4 mm, clockwise) to capture as much analyte as possible. To consider the effects of the sample introduction method (*i.e.,* wipe-based samples and OPSI extraction), solution standards were also analyzed at equivalent mass loadings (five replicates each) by direct pipetting into the OPSI solvent dome. The system yielded mostly nonlinear response curves exhibiting signal saturation in the higher mass range for both wipe-based and direct solution pipetting samples. Signal saturation in ESI-MS at high flow rates and concentrations is well documented in the literature.45, 46

OPSI-MS sensitivities for each of the target analytes were established for both wipe-based samples and direct solution samples. The limits of detection corresponding to the mass yielding 90 % probability of true detection (LOD90) were determined as specified by ASTM E2677 (Standard Test Method for Determining Limits of Detection in Explosive Trace Detectors).47 Table 1 displays the LOD90 values for each sample and sample introduction method (exact wipe-based sample LOD90 values were obscured with order of magnitude values for security purposes). The wipe-based samples yielded single-digit nanogram to sub-nanogram detection limits. In comparison, the solution-based samples (direct pipetting into solvent meniscus) yielded more sensitive LOD90 values by a factor of 2 up to a factor of 35. The improvements clearly indicated inefficiencies in sample extraction from the wipe substrate. Inefficiencies might have resulted from poor analyte dissolution in the chosen solvents, incomplete interaction and extraction, or wicking and transport of dissolved analyte across the wipe instead of to the ESI source (material losses).

**Table 1**. OPSI-MS detection of organic explosives, inorganic oxidizers, and a narcotic. Data includes dominant observed ion, LOD90 values (calculated according to ASTM E2677) and signal decay time constants (taken at 1000 ng loadings).

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Compound** | ***m/z*** | **Observed Ion** | **Wipe LOD90 (ng) a** | **Solution LOD90 (ng) b** | **Wipe Decay Time Const. (s)** | **Solution Decay Time Const. (s)** |
| **RDX** | 280.9 | [M+CH3COO]- | < 1 | 0.11 | 20.2 ± 8.9 | 2.7 ± 0.1c |
| **TNT** | 225.9 | [M-H]- | < 10 | 0.19 | 23.1 ± 7.2 | 4.1 ± 1.1 |
| **PETN** | 374.9 | [M+CH3COO]- | < 1 | 0.21 | 9.9 ± 3.8 | 2.9 ± 0.5 |
| **NaNO3** | 61.9 | NO3- | < 10 | 0.49 | 12.9 ± 7.5 | 3.3 ± 0.5 |
| **KClO3** | 83.0 | ClO3- | < 1 | 0.20 | 19.2 ± 7.6 | 3.3 ± 0.5 |
| **KClO4** | 99.0 | ClO4- | < 10 | 0.14 | 23.3 ± 14.3 | 2.9 ± 0.6 |
| **Cocaine** | 304.2 | [M+H]+ | < 1 | 0.17 | 8.2 ± 1.2 | 3.3 ± 0.1 |

a Exact LOD90 measurements were approximated for security purposes.

b Solution LOD90 are approximate. Full ten replicates needed for ASTM E2677 were not available.

c Decay time constants were taken from 300 ng data for RDX.

**Temporal Response**

With the initial characterization of the OPSI-MS ion distributions and sensitivities of the target analytes, we further investigated the sample introduction process effects on the temporal response. First, the transit time for sample from the OPSI, through the ESI source, into the mass analyzer, and to the detector was estimated. Direct solution-based sample pipetting into the OPSI solvent meniscus resulted in approximate transit times of 2 s to 3 s. The duration of each signal was a strong function of the sample introduction method and sample mass. Figures 2A and 2B display representative extracted ion chronograms for potassium chlorate (selected ion monitoring of ClO3-) from wipe-based samples and direct pipetting of solution-based samples. Direct solution introduction yielded increasing self-similar signal profiles, much as expected for introduction of a near instantaneous sample plug into laminar capillary flow. The observed asymmetrical nature of the peak and tailing were a result of Taylor-Aris dispersion.48

Visually, the extracted ion chronograms for the wipe-based samples extended across much longer time scales (*i.e.,* around 8 s up to > 45 s) relative to the solution-based samples (*i.e.,* full width at half maximums of around 5 s). The response to wipe-based samples most frequently resulted in an initial peak in signal followed by a protracted decay with numerous local maxima and minima (Figure 2A). The maximum peak intensity and overall signal duration increased as a function of increasing analyte mass. Wipe-based samples clearly introduced an additional ‘extraction’ time that contributed to these profiles. In addition, wipe-based samples also experienced prolonged signal due to sample ‘searching’ (*i.e.,* moving the wipe around). The relative sizes of the OPSI extraction area (≈ 4 mm solvent dome diameter) and wipe collection area (≈ 1.5 cm diameter) required manual manipulation of the wipe-OPSI interaction around this central sample deposit area. In addition, the sample spot size (*i.e.,* effective particle diameter) was orders of magnitude smaller than the OPSI solvent dome. As the wipe moved around, the dissolving particle could be right in the middle of the OPSI and immediately transported toward the ESI-MS, and then move out near the periphery and yield delayed transport. These additional aspects of wipe-based OPSI sampling also increased the uncertainty in replicate measurements as demonstrated by the relative standard deviations in Figures 1E, 1F, and S1. Figures 2C and 2D show representative replicate measurements for wipe-based and solution-based 100 ng TNT samples. Direct solution pipetting into the OPSI yielded very repeatable measurements with a relative standard deviation (RSD) of 4 %. Alternatively, the wipe-based TNT samples yielded an RSD of 34 %. RSD’s were calculated from peak area integration (*i.e.,* signal above baseline) during wipe exposure of replicate measurements.

Due to the importance of rapid analysis and cleardown (*i.e.,* returning to baseline conditions) for trace detection applications in screening environments, we quantified the signal decay of both sample sets by fitting to a simple exponential function, , where *Io* is the maximum intensity and τ is the decay time constant (Figures 2C and 2D insets). Signal decay time constants were determined for the highest mass loading investigated here (*i.e.,* 1000 ng) and are displayed in Table 1. The solution samples decayed rapidly, with an average decay time constant of around 3 s across the target analytes. The self-cleaning nature of the OPSI source demonstrated minimal contamination or carryover (Figure S3: extracted ion chronograms and total ion current chronograms of replicate wipe-based samples).34 Comparatively, the wipe-based samples exhibited decay time constants from around 8 s to 23 s, with sample-to-sample variability in time constant up to 60 % RSD. It is important to note that this study sought to provide a preliminary characterization of coupling the OPSI-MS system with wipe-based sample introduction, common to swipe sampling screening applications. Here, we focused on understanding this sample introduction mode relative to direct solution introduction and on quantifying system sensitivity. Therefore, we aimed to completely extract and fully detect the available sample on each wipe. However, from a screening standpoint, only sufficient signal for an alarm might be necessary, potentially at the maximum peak intensity. The maximum peak intensity generally occurred within 5 s to 8 s of sample introduction for the wipe-based samples (Figure 2).



Figure 2. Representative extracted ion chronogram profiles of potassium chlorate (*m/z* 83 ClO3-) as a function of increasing mass (1 ng, 10 ng, 30 ng, 100 ng, 300 ng, and 1000 ng) for (A) wipe-based sample introduction and (B) direct pipetting into the OPSI. Insets: schematics of sample introduction modes. Replicate extracted ion chronogram profiles for 100 ng samples of TNT (*m/z* 226 [TNT-H]-) for (C) wipe-based sampling introduction and (D) direct pipetting into the OPSI. Insets: demonstrations of signal exponential decay fitting for 1000 ng potassium perchlorate (*m/z* 99 ClO4-) samples.

**Sampling Substrate, Polarity Switching, and Mixtures**

Thus far, we have completed all analyses using a PTFE-coated fiberglass weave wipe, common to a number of commercial IMS systems and swipe sampling applications. Next, we briefly considered the effects of sampling substrate with comparison to another common material, *meta*-aramid Nomex. Figures 3A and 3B compare the OPSI-MS response of 100 ng RDX and 100 ng potassium perchlorate as a function of wipe material. The RDX samples exhibited a significant (95% confidence) reduction in peak area of *m/z* 281 [RDX+OAc]- for the *meta­*-aramid Nomex wipes. Alternatively, the potassium chlorate samples did not exhibit the same signal decrease, with the median peak area of the perchlorate anion (*m/z* 99 ClO4-) remaining the same (within 95 % confidence). Initially observations attributed this to wicking of solvent and target analyte away from the OSPI port inlet, resulting in material loss. The *meta*-aramid Nomex wipes were a more fibrous material that demonstrated substantial solvent wicking for the acetonitrile/water (95/5, v/v) base solvent used for organic compounds. The wicking effect, sample loss, and resulting signal reduction was attenuated when increasing the water composition up to 50/50 (v/v, acetonitrile/water) for the inorganic oxidizers. The liquid-based nature of sample extraction in OPSI-MS (as opposed to traditional thermal desorption) requires consideration of a different set of parameters for wipe optimization (*e.g.*, solvent resistance, hydrophobicity, porosity, and capillary action).

The analysis of target compounds in both positive and negative polarity mode operation is another central aspect to high throughput screening. Most screening arenas target explosives, which include nitramines, nitroaromatics, and nitrate esters commonly found in negative mode, and peroxides commonly found in positive mode. High throughput screening is also frequently used for narcotics screening, which are often preferentially found in positive mode. We conducted a brief look at analyzing samples containing both 100 ng RDX and 100 ng cocaine with a polarity switching method with a 5 millisecond pause between each positive scan and negative scan. Both target compounds were clearly identified in their preferential ionization modes. Figures 3C and 3D compare the dominant ion peak areas for each analyzed with a single polarity method and the polarity switching method. RDX demonstrates a slight increase in peak area distribution for replicate measurements, however, the median peak areas were statistically the same (95% confidence). Contrarily, cocaine demonstrated a significant decrease in median peak area (95% confidence) for the polarity switching method. This decrease was likely the result of front-end contamination and charging effects from the 10 mmol/L ammonium acetate component of the OPSI solvent. Ongoing work is considering optimization of the OPSI solvent to maximize extraction of both organic and inorganic species and minimize charging effects in potential polarity switching mode operation.

Finally, we demonstrated the analysis of a complex mixture, specifically, a black powder substitute propellant, with the OPSI-MS system. Perchlorate (*m/z* 99 ClO4-), perchlorate dimer (*m/z* 199 (HClO4)(ClO4)-), and a potassium perchlorate-perchlorate adduct (*m/z* 237 (KClO4)(ClO4)-) were readily observed in the mass spectra of the Jim Shockey’s Gold propellant (a commercially available black powder substitute) samples (Figure S1). In addition, minor peaks for degradation products of the propellant fuel, ascorbic acid, were also observed, including, oxalic acid (OA: *m/z* 89 [OA-H]-) and threonic acid (TA: *m/z* 135 [TA-H]-). Ascorbic acid degradation in solution has been demonstrated in the literature and expected here given the nature of OPSI-MS.49, 50



**Figure 3**. Box-whisker plots of peaks areas for inkjet printed wipe-based samples analyzed by OPSI-MS. Comparisons of (A) 100 ng RDX: *m/z* 281, [RDX+OAc]- and (B) 100 ng potassium perchlorate: *m/z* 99, ClO4- responses for PTFE-coated fiberglass weave and *meta-*aramid Nomex wipe materials. Comparisons of (C) 100 ng RDX: *m/z* 281,[RDX+OAc]- and (D) 100 ng cocaine, [cocaine+H]+ responses for single polarity and polarity switching methods. Boxes, whiskers, and outliers (**+**) signify median ion ratio with lower and upper quartiles, 1.5× interquartile range, and ratios beyond that range. Open circles represent data points and triangles represent the 95% confidence intervals around each distribution’s median.

**Conclusions**

This preliminary investigation of OPSI-MS demonstrated a versatile platform for trace contraband detection. Traditionally in screening settings, multiple techniques are employed for the detection of both organic and inorganic target threat compounds. Analytical techniques have long been striving for improved and combined organic/inorganic detection methods. The liquid dissolution and extraction nature of the OPSI interface enabled sampling of both organic explosives and nonvolatile inorganic oxidizers common to homemade explosives in a single analytical platform. Coupled to a compact single quadrupole mass spectrometer, the system exhibited several nanogram to sub-nanogram sensitivities. However, these sensitivities were measured on pure compounds under ideal laboratory conditions. This study did not address performance under deployed settings or analysis of samples collected under real-world settings. These aspects would limit sampling time, yield poor(er) sampling efficiency, introduce background interferences, and matrix effects. Therefore, no direct conclusions were drawn regarding applicability to real world screening arenas. These questions will be examined in a follow-up publication. Future work may also improve upon detection limits with optimization of the extraction solvent to maximize analyte solubility or through enhanced ionization with specific additives. This study also demonstrated the need for improving the repeatability of OPSI extraction-to-wipe sampling area interaction. Given the typical collection area of swipe sampling techniques, increasing the overall OPSI extraction area, automating sample rastering (*e.g.,* spiral search), or creating targeted localization of the sample collection (*e.g.,* topographical slits to spatially control sample location) could reduce variability and unnecessary manual sample “searching” delays. Methods to optimize the user-controlled wipe-to-solvent dome interaction are also needed. From a screening application standpoint, complete extraction of the available sample is not required, rather just sufficient signal for alarm. Therefore, immediately bringing the collected sample into contact with the OPSI solvent meniscus may prove beneficial. Ongoing and future work aim to explore these areas, additional system parameters, and further mixture analysis, potential signal suppression, and other matrix effects.

Author Contributions

TPF: Conceptualization, Formal analysis, Visualization, Writing – original draft, review, and editing. JL: Investigation, Resources, Writing – review and editing. CH: Investigation, Methodology, Resources, Writing – review and editing. GG: Conceptualization, Funding acquisition, Methodology, Supervision, Writing – original draft, review, and editing. All authors have read and approved the final version of the manuscript.

**Conflicts of interest**

There are no conflicts to declare.

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