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Analytical Validation and Impact Assessment of On-Site Evidence Screening via Ambient Sampling, Portable Mass Spectrometry

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Final Summary Overview

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Statement of Purpose

Forensic evidentiary backlogs are indicative of the growing need for cost-effective, high-throughput instrumental methods. One such emerging technology that shows high promise in meeting this need, while also allowing on-site investigation, is portable mass spectrometric instrumentation, particularly that which enables the coupling to rapid, ambient ionization methods. Such technology has the potential to assess the probative value of chemical evidence at the crime scene, requiring only pertinent samples to be sent to off-site laboratories for confirmation, easing the burden of casework and therefore reducing the magnitude of backlogged evidence. Screening of physical evidence at the crime scene also has the capability to rapidly determine whether a criminal investigation is needed and provide law enforcement personnel with necessary information in a timely manner, which in many cases is crucial.

Through National Institute of Justice funding, an interdisciplinary team of researchers developed direct evidence screening methods on a commercially-available, portable mass spectrometer (MS), culminating in a fieldable instrument that is simplistic in operation, yet robust to the needs of today's forensic and law enforcement practitioners. Emerging drug classes and authentic evidence types were investigated on the system in order to show robustness to the influx of novel psychoactive substances (NPS) seen in illegal drug seizures. A rigorous analytical validation using common illicit chemicals was also performed to ensure that reliable and reproducible usage by non-technical operators is feasible and to facilitate future court admissibility of field-collected forensic data. A significant aspect of this project was designed not just to anticipate, but to predetermine the legal and economic impacts of adopting this technology for field usage to inform and help guide forensic science policy and practice. In an effort to predetermine legal implications of adopting this technology for field use, the current state of U.S. search and seizure law was examined to recommend legal investigation strategies by law enforcement, including the potential legality of using this technology to prompt a "probable cause" search. To assess the financial viability of instrument-based analysis of forensic evidence in the field, fiscal-impact models were created to compare this proposed methodology to the current system of off-site evidence processing at publicly-funded laboratories in terms of both cost and processing time.

Project Design and Methods

The project discussed herein was designed to assess feasibility, analytical performance, anticipated legality of field usage, and the economics of broad implementation of portable MS systems featuring simplified sample handling methods. To effectively address these broad research directions, an interdisciplinary approach was taken, breaking down objectives into three main streams: *analytical characterization and validation*, *determination of legal investigative strategies*, and *financial viability of deployment.* Principal research questions addressed during this work were as follows: **(i)** Can the proposed technology be adapted for routine and reliable usage by non-technical operators? **(ii)** Is the analytical performance of the technology on par with current methods for forensic evidence processing? **(iii)** Can the technology be used to prompt "probable cause" searching by law enforcement in innovative, yet legal, ways? **(iv)** What are the financial benefits of the proposed technology in comparison to current practices?

Analytical Characterization and Validation

Portable MS System and Paper Spray Ionization – Mass Spectrometry (PSI-MS)

The portable MS system employed for this research was the FLIR Systems AI-MS 1.2 cylindrical ion trap mass spectrometer (Figure 1), which offers both ruggedness towards field conditions and tandem MS analysis for increased selectivity of chemical identification. Through past NIJ funding (NIJ Grant No. 2011-DN-BX-K552, end date: 12/31/2014), this system was shown to be applicable to a myriad of forensic chemicals and evidence types, with particular proficiency in illicit drug identification. Further, the AI-MS 1.2 allows for "red light/green light" operation, alleviating the need for user-based data analysis by employing automated chemical identification based upon an on-board spectral database.

This system can also be coupled with ambient ionization methods, which in turn allows the analysis of forensic evidence in its native state, with little to no preparation necessary; alleviating sample preparation increases both the sample throughput and simplicity of operation by non-technical operators. Past grantwork showed that paper spray ionization (PSI) had especially high proficiency for common and emerging drug evidence types, allowing the quick screening of both bulk illicit substances and trace residues via surface transfer swabbing. Shown in Figure 2, PSI utilizes a paper substrate as both the

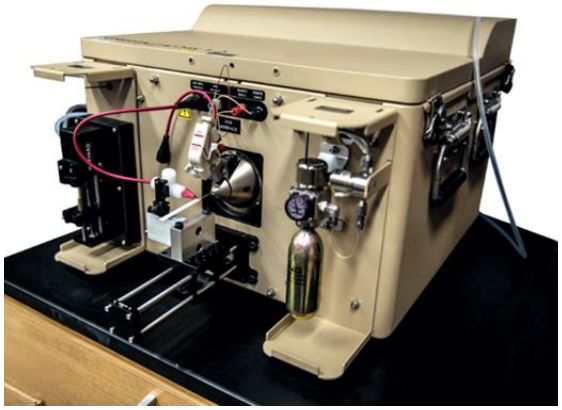

Figure 1. FLIR Systems AI-MS 1.2 portable, ambient sampling mass spectrometer (MS). This simplified, ruggedized instrument allows users to perform mass analysis and automated chemical detection directly from surface swabs in the form of paper spray ionization (PSI).

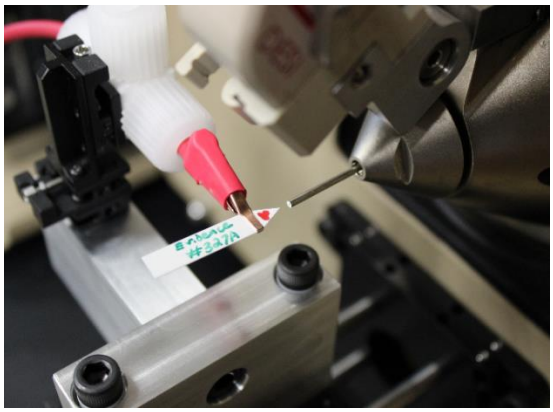

Figure 2. Simplified paper spray ionization (PSI) source implemented on the AI-MS 1.2 portable MS system. Chemical analysis is performed directly from a triangular paper swab after addition of solvent and voltage. Said swab can be used to dip-test forensic evidence or implemented as a surface swab.

sampling apparatus and the disposable ionization source. Simple application of solvent and high voltage allows the analysis of surface-bound analytes.

Categorical Validation of PSI-MS on the FLIR AI-MS 1.2

In an effort to both characterize the portable MS methodology and facilitate future court admissibility, an extensive analytical validation was undertaken, following recommended guidelines set forth by the Scientific Working Group for the Analysis of Seized Drugs (SWGDRUG). Specific performance characteristics examined included selectivity of chemical identification, accuracy/precision, PSI method robustness, environmental ruggedness, and trace evidence detection limit. Reliability in the form of false positive/negative response rates for drug controls were determined from experiments with large sample sizes ($n > 1000$), examining the effect of user training and experience level. Environmental factors stemming from field usage, including wind speed and direction, relative humidity, and ambient temperature, were also investigated, assessing the effect on duration and intensity of mass spectral data.

Legal Investigative Strategies Using Portable MS Systems in Law Enforcement Activities

The goal of this research stream was to review current and past case law in order to identify verdicts and discourse that could set precedent on how, and under what circumstances, portable MS evidence screening could be utilized in law enforcement activities. Of particular interest was case law involving the

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use of new technologies by law enforcement (*e.g.* thermal imaging, GPS location tracking, portable contraband screening), as well as the various warrant exceptions to the Fourth Amendment and how they may relate to field usage of portable MS systems. To thoroughly explore the lineage of these cases, *Shepard's Citations,* a tool that identifies all subsequent court decisions that cite the precedent being studied, was used to provide a comprehensive examination of how lower courts have treated these legal precedents. To elucidate interrelation between these cases, Max QDa qualitative data analysis software was utilized. Using the current state of the law interpreted from these results and considering recent changes to the membership of the U.S. Supreme Court, tactical recommendations for legal usage of portable MS systems in law enforcement activities were crafted.

Financial Viability of Portable MS Deployment

Adopting instrument-based methods for field evidence screening represents a major expenditure, so it is prudent to consider its economic impact. To this end, a flexible fiscal impact model was developed to assess the financial viability of implementing portable PSI-MS systems in crime scene and law enforcement scenarios for drug evidence screening. This model estimates the costs per sample for both traditional evidence processing (*i.e.* off-site analysis in the public crime lab system) and portable MS-based processing across all phases of forensic evidence collection and analysis: (i) on-site costs, (ii) precinct-born costs, (iii) evidence transport costs, and (iv) in-lab costs. Data inputs specific to PSI-MS on the AI-MS 1.2, such as consumables cost and sample throughput, were directly determined from replicate investigations of illicit drugs. Data inputs associated with evidence collection, handing/documentation, transportation, and crime laboratory analysis were estimated from police and forensic lab practitioner interactions, publicly-available, web-based data from state forensic labs, and the scientific literature.

Sensitivity analyses were performed to determine which input variables most significantly impacted cost per sample. Monte Carlo stochastic simulation was used to account for uncertainty in the model inputs that were identified as sensitive or highly variable (*e.g.* labor costs/salaries). Here, random number generators produce a range of values for the model inputs, which are modelled as random variables with representative probability distributions. Ultimately, this allows for a more accurate estimate of the costs per sample for the current and proposed processes. The simulation output allows for estimating not only the

average costs per sample, but also the standard deviation, confidence intervals, and the entire empirical distribution, if needed.

Project Findings

Validity and Applicability of Portable MS Processing of Forensic Evidence

The validation plan implemented for the FLIR AI-MS 1.2 was constructed to include performance characteristics delineated in recent SWGDRUG recommendations (Vers. 7.1) for seized drug analysis methods. Specific categories incorporated were *sample throughput*, *selectivity* of analyte identification, *accuracy/precision* (*i.e.*, repeatability, inter-user reproducibility, and error rate), *method robustness* of PSI-based evidence screening, *environmental ruggedness*, and *detection limit* for trace residues.

Sample throughput rates were systematically determined for various user classes (*e.g.* experienced vs. non-experienced, physical science background vs. non-technical operator, etc.) to be 4 minutes/sample or less, depending on cumulative, on-system experience. Selectivity of spectral-based chemical identification was shown to be high, even for structurally-similar compounds, by comparison to the Wiley Registry of Tandem Mass Spectral Data. While collected data exhibited significant inter-day and inter-user variability in regards to the spectral intensity observed, the reliability of detection was shown to be relatively unaffected when investigating low complexity samples. PSI screening on the AI-MS 1.2 was conducted on ~ 1200 (each) positive and negative drug control samples, yielding a true positive detection rate of 99.01% and false positive detection rate of 0.17%; these rates obtained suggest that reliable field-based chemical evidence screening can be accomplished even when operated by non-technical users. As part of environmental ruggedness validations, a systematic study of wind speed/direction, relative humidity (%), and ambient temperature was conducted. While signal intensity and duration was shown to be affected by broad seasonal ranges of temperature and humidity, false positive/false negative rates remained constant. Wind speed and direction were shown to increase error rate, but only when wind speed surpassed 5 m/s (11.2 MPH). Detection limits ranged from low nanogram to low microgram for drug residue screening, depending on specific chemicals and surfaces investigated, supporting the use of PSI-MS for trace evidence analysis.

While recent advances in the fields of ambient and portable mass spectrometry have intrinsic value in combatting the growing forensic evidentiary backlog, this work represents the first multi-category analytical validation of a field-ready system. Validation categories examined, particularly selectivity, error rate, and ruggedness, will assist in meeting the demands of the Daubert standard for future admissibility of field-collected MS data.

Through the project lifetime, significant effort was taken to demonstrate broad applicability of portable MS evidence screening towards novel drug classes, evidence types, and investigative scenarios. As a deliverable, a spectral library of PSI-MS and MS/MS data was produced from novel synthetic cannabinoids and phenethylamines to shown application to emerging drug trends. Application to abused pharmaceutical tablets (*e.g.* Adderall, etc.), fentanyl, and α-PVP was also demonstrated. Through interactions with local and state-level law enforcement, authentic evidence was also successfully processed on the system, such as bulk methamphetamine, synthetic marijuana, and purported MDMA, as well as novel paraphernalia types (*e.g.* NBOMe derivatives on blotter paper, beverages spiked with codeine-based cough syrup, and adulterated electronic cigarette liquids). The proficiency of detecting trace drug residues from latent fingerprints via surface swabbing and PSI-MS was also shown, which was examined as an interesting investigative strategy in routine traffic stops.

Recommendations Regarding Portable MS Usage in Law Enforcement Activities

Recommendations as to the criminal justice policy impacts of evidence screening via portable MS and its possible field usage were developed after a thorough review of all relevant Supreme Court decisions and other literature regarding the use of new technologies and narcotic detection dogs in law enforcement activities involving potential search and seizures. Of note, it is anticipated that once a criminal activity/crime scene has been identified or probable cause for a warrantless search during enforcement activities is established, the use of portable MS systems as a forensic tool to process potential evidence would enjoy full legality. However, the use of chemical information stemming from this implementation as expert testimony in the court setting would be contingent on adherence to the Daubert (or Frye) standard. Furthermore, the usage of portable MS for contraband screening in a correctional setting, where inmates

have minimal or no privacy rights from being under state or federal supervision, would also have a sound legal basis.

The content analysis revealed the reliability of narcotic detection dog "sniffs" as being a critical question needing exploration to evaluate parallels to portable MS use in activities of more nebulous legality, such as establishing probable cause for a vehicle search during traffic stops. An analysis of 57 decisions showed that most courts have found detection dogs as reliable, as long as they were formally trained and certified. Only a handful of lower courts were even critical of arguments that dogs were improperly "cued" by their handlers to encourage an alert, or had a tendency to make "false alerts" in which no contraband was found.

The high selectivity of chemical identification and low false positive/false negative rates established through this grant work suggest that portable MS screening would be considerably more reliable than dog sniffs, and it could enjoy similar jurisprudence. Efforts and insights from this phase of the project were used to craft a deliverable recommendation regarding legal investigative strategies of portable MS systems. In summary, said recommendation distinguishes a range of scenarios in which the use of portable MS systems would be constitutional, posing no legal barriers. These include: using the portable MS system to determine probable cause in a traffic stop, through mechanisms such as screening external vehicle surfaces and latent fingerprints on identifying materials of a driver (*e.g.* licenses and registration cards); in cases involving abandoned property; and in specific exigent circumstances, such as recording the presence of contraband when there was a real risk of evidence destruction. Correspondingly, portable MS systems are not suitable, nor recommended, for implementation prior to establishing probable cause in the contexts of the trespass doctrine (*i.e.* the curtilage of a residence), during "stop and frisk" scenarios that are limited to pat-downs for weapons, or in inventory searches of impounded vehicles.

Financial Viability Recommendations Regarding Field Usage of Portable MS Systems

Using the generated fiscal impact model, several usage modes of portable MS evidence processing were examined in an effort to determine cost effectiveness. For example purposes, the usage modes examined here include using portable MS for presumptive testing, combining portable MS data with a

targeted, Category A analysis at an off-site laboratory to meet SWGDRUG recommendations of two-tiered testing, and combining portable MS screening with colorimetric field tests for confirmatory analysis.

Table 1 shows the comparison of these specific usage modes to traditional, forensic laboratory-based evidence processing (*i.e.* "current process") in regards to crime scene investigation. Variable and fixed (*e.g.* lab instrumentation acquisition/maintenance) costs are itemized and used to compute average total cost per sample. Then, after incorporating uncertainty with regards to the input variables via Monte Carlo simulation, 95% confidence intervals can be determined for a more accurate estimate of the total cost per sample for evidence processing and analysis.

Table 1. Example model output comparing current and proposed processes for crime scene scenarios

Costs per Sample	**Current Process**	**Presumptive AIMS**	**Targeted Cat. A**	**Confirmatory Color Test**
(1) Average On-Site Costs	$5.31	$10.40	10.40	$18.28
(2) Average Precinct Costs	$6.46	$6.46	$6.46	$6.46
(3) Average Evidence Transport Costs	$22.72	$21.71	$21.27	$5.43
(4) Average In-Lab Costs	$115.86	$69.61	$59.80	$39.06
Fixed Cost Per Sample for Necessary In-Lab Instrumentation Use	$16.63	$10.08	$10.08	$2.44
Average Total Cost Per Sample and	**$166.98**	**$118.26**	**$108.01**	**$71.67**
Standard Deviation	$12.55	$8.05	$7.20	$6.50
95% Confidence Interval	($167.52 - $172.44)	($116.68 - $119.84)	($106.60 - $109.42)	($70.40- $72.94)
Expected Cost Reduction	---	**29%**	**35%**	**57%**
Breakeven Point	---	**646**	**534**	**330**

For these results, it is important to note that fixed costs related to portable MS acquisition/maintenance and training are not incorporated in the total cost per sample. Alternatively, we calculate the minimum number of samples requiring analysis per year to recoup the total fixed cost of purchasing and maintaining a single AI-MS 1.2 system (~ $295,000 over the expected lifetime), which is referred to as the *Breakeven Point*, based upon expected cost reductions of the specific usage modes.

The breakeven points generated from the fiscal-impact model are intended to guide decision-makers and forensic practitioners in assessing whether incorporation of field-based AI-MS 1.2 units are financially-viable and logistically suitable for their intended use and enforcement needs. Model outputs can also be utilized to consider both small and large scale implementation. Table 2 shows extrapolated cost savings for the example usage modes for the processing of 10,000 evidence samples, which is representative

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based on per capita drug evidence requests for a large urban area. Then, considering fixed costs related to the AI-MS 1.2, expected cost savings per year are calculated for varying numbers of systems employed. As seen, depending on the fleet of systems used and the usage mode, a significant cost savings can be realized. However, this assumes that the municipality or jurisdictional area requires that magnitude of drug evidence per year and can support that level of usage over the estimated lifetime of the instrumentation. Likewise, if the jurisdictional area is a large urban center with a modest crime rate, the total number of instruments employed must be suitable from a logistical standpoint to be useful.

Table 2. Expected cost savings per year for high volume processing of forensic evidence via portable MS

Scenario: Mid-to-Large Urban Area	Current Process	Presumptive AIMS	Targeted INA1	Confirmatory Color Test
Evidence Samples per Year	10,000	10,000	10,000	10,000
Total Cost Per Sample (calc.)	$169.98	$118.26	$108.01	$71.67
Total Costs Accrued for Analysis per Year (Minus AI-MS 1.2 Fixed Costs)	$1,699,800	$1,182,600	$1,080,100	$716,700
No. of AI-MS 1.2 Systems Employed:	**Expected Cost Savings Per Year (All Costs)**			
1	---	$455,721	$558,221	$921,621
5	---	$329,807	$432,307	$795,707
10	---	$172,414	$274,914	$638,314
15	---	$15,021	$117,521	$480,921
20	---	$-142,372	$-39,872	$323,528

Along with the fiscal impact model, recommendations regarding the most cost-effective usage modes of portable MS systems were crafted, in which detailed explanations of model input/outputs and simulation strategy are given. As some aspects of the usage modes examined may be incongruous in regards to specific municipal and state drug enforcement policies, financial recommendations are presented so that decision-makers can use their discretion in assessing impact. As a whole, usage scenarios that increase the overall magnitude of evidence processed per portable MS instrument employed while minimizing the need for off-site processing via forensic laboratories are postulated to be the most cost-effective, and in some cases, cost savings are anticipated.

Implications for Criminal Justice Policy and Practice

While a significant portion of this proposal is designed to predetermine the legal and economic impacts stemming from adopting portable MS technology for field usage, certain aspects can be anticipated. The flexibility to screen and identify forensic analytes present in various states and matrices on-site via PSI

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has the potential to provide capabilities that no other fieldable technology currently available offers. In the interest of public safety, it is essential that forensic practitioners and law enforcement agencies are provided with the suitable, yet fiscally responsible, equipment to effectively perform their duties. When considering the end-product of the research proposed, a portable instrument capable of assessing the probative value of physical evidence typically found at crime scenes, the impact of providing the forensic science community with said technology would have a positive effect on criminal justice practice at the local, state, and national level. A reduction in the current backlog of forensic evidence could come from two improvements to forensic science, higher throughput analytical techniques or a reduction of the influx of evidence to forensic laboratories. Portable MS systems featuring ambient ionization methods like PSI are capable of both.

The deliverable legality and economic recommendations generated as part of this work are designed to help inform and guide forensic science policy and practice. The policy contributions proactively anticipate the legality of the various usage modes of this methodology, particularly in regards to Fourth Amendment rights, and the analytical validation efforts will help to evaluate the admissibility and refutability of field-collected data on the FLIR AI-MS 1.2 in the court of law. The financial viability research helps to anticipate the costs and potential savings from both small and large-scale implementation of field-portable MS units. When considering the feasibility of implementing the proposed technology in forensic and law enforcement settings, the cost of instrumentation, training and maintenance could be off-set by the reduction in evidence sent to forensic laboratories and funds being used for outsourcing analyses to private laboratories. Field screening of forensic evidence could alternately allow reallocation of publicly-funded forensic lab resources to other areas of need, such as the current backlog of DNA and other biology requests, as well as potentially reduce jailing and litigation expenditures through increased plea-bargaining rates. Besides utility towards the proposed research, the fiscal-impact model constructed through this project can serve as the boilerplate for assessing the financial impacts of future technologies.

To date, dissemination of project findings to the greater forensic, criminal justice, and simulation communities has occurred on multiple fronts in order to maximize impact, including four (4) peer-reviewed publications, twenty-four (25) presentations at national and regional conferences, and demonstrations/interactions with local and state policing agencies.