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Overview of Report

The National Institute of Justice (NIJ)'s Forensic Technology Center of Excellence (FTCoE) at RTI International worked with law enforcement (in areas such as mail safety, hazardous materials, and homeland security), the forensic community, and various instrument manufacturers to perform this landscape study of portable and handheld devices that can be used for presumptive drug testing of controlled substances in the field.

A landscape study provides a comprehensive overview of market participants, their products, and product features to enable end users to make better-informed purchasing decisions. This report gives an overview of currently available methods and technologies for field-based presumptive drug testing beyond traditional color-based testing.

The FTCoE cautions that those considering the implementation of field portable devices for presumptive drug testing should abide by their agency's policies and procedures regarding drug interdiction efforts. Drug testing in a field setting, regardless of the technology employed, may expose law enforcement officials to potentially harmful substances.

The following factors led the FTCoE to conduct a landscape study of field testing devices:

- ► There has been an alarming rise in the incidence of dangerous substances, such as fentanyl analogs, emphasizing the need for increased safety measures. New field testing techniques could address and minimize hazards to individuals in the field.
- New drugs, such as novel psychoactive substances, are hitting the streets every day. Development of color-based tests may not keep up with these types of drugs, but alternative, more robust technologies may improve the process of rapidly identifying these substances.
- ► Multiple types of portable presumptive field drug testing devices are available in the market, which makes it difficult for decision makers to choose the most appropriate instrument.

Objectives of Landscape Study

This document provides decision makers and end users, such as law enforcement officers, drug unit members, and other stakeholders, with the following:

- Overviews of the multiple roles of presumptive drug testing in the field, including past and current methods and technologies used.
- Specifications on available products from selected manufacturers.
- Insights from current users to inform potential technology adopters about implementation considerations for portable field testing devices.
- Discussion of the benefits, limitations, and implementation considerations for various technologies, including mass spectrometry (MS), ion mobility spectrometry (IMS), portable Raman spectroscopy, infrared spectroscopy (IR), and color-based testing techniques.
- Cases illustrating the successful adoption of new and upcoming field testing techniques.

This study informs potential end users about the multitude of options for field drug testing that could help to increase safety, decrease time spent at a scene, potentially decrease backlogs, and facilitate legal proceedings. Field testing of novel psychoactive substances (NPSs) is also discussed in-depth, as the need for NPS testing continues to escalate.

Landscape Methodology

To conduct this study, the FTCoE used a process that included the following steps:

- Consulted secondary sources—including journal and industry literature—to obtain information related to field testing devices, successful use cases, and procurement considerations for the devices.
- Discussed current presumptive drug testing techniques with subject matter experts, including crime scene and laboratory practitioners, law enforcement officers, technology developers, legal professionals, and key decision makers.
- Visited the Edgewood Chemical Biological Center (ECBC) to better understand certain technologies, obtain firsthand experience with instrumentation, and discuss technology benefits and limitations with users.
- Documented, summarized, and released key findings (by way of this report) to the forensic community.

Subject Matter Experts and Stakeholders

We would like to thank the various forensic science community stakeholders and practitioners who offered insight and expertise.

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Glossary of Commonly Used Words and Phrases

For the purposes of this document, the following terms are defined [1]:

Adulterant: a compound added to a substance, such as an inert cutting agent or other active drugs.

ASTM: American Society for Testing and Materials.

Carrier gas: an inert gas used in chromatography to "carry" the solutes through the column.

Chemical structure: the spatial arrangement of atoms in a molecule and the number, type, and location of chemical bonds between atoms [2].

Confirmatory drug test: a test that allows for structural identification of a drug.

Controlled substance: a drug or other substance for which manufacture, possession, or use is regulated. In the United States, controlled substances are those that are included in one of the five schedules of the controlled substances act (CSA).

Controlled substance analog: a substance that is not explicitly named in controlled substance regulations but is substantially similar to one that is. In the US, any substance that meets the legal definition of a controlled substance analog (21 U.S.C. §802(32)(A)) is treated as a controlled substance.

Cutting agent: a chemical that is usually inexpensive, easy to obtain, and may replicate the physical attributes of the drug that is being adulterated, such as baking soda.

Functional group: a group of atoms responsible for the characteristic chemical reactions of a particular compound, such as the N-methyl (amine) group in morphine.

Interference: a signal produced by a non-target analyte that affects the signal from the target analyte.

Isomer: each of two or more compounds with the same molecular formula but a different arrangement of atoms.

Molecular Formula: the number of each type of atom in a molecule (e.g., $C_{17}H_{19}NO_3$ is the molecular formula for morphine).

Novel Psychoactive Substance (NPS): a typically synthetic compound that produces effects similar to those of traditional drugs, such as opioids, cathinones, and cannabinoids.

Presumptive drug test: a test that indicates the presence of a drug.

Roughing pump: a vacuum pump used to lower the pressure in a mass spectrometer.

Selectivity: the ability of a test to distinguish a target analyte from other analytes.

Sensitivity: the ability of a test to detect the target analyte.

Solid-phase microextraction (SPME): a solvent-free technique using a polymer-coated fiber to extract analytes of interest through absorption prior to chromatographic analysis.

SWGDRUG: Scientific Working Group for the Analysis of Seized Drugs.

SWGDRUG category: a classification system for the discriminating power of analytical techniques. Category A comprises the most discriminating techniques, Category B techniques are less discriminating than those in Category A, and Category C contains the techniques that are the least discriminating.

Thermally labile: refers to a compound that may be altered or destroyed upon exposure to heat or high temperatures.

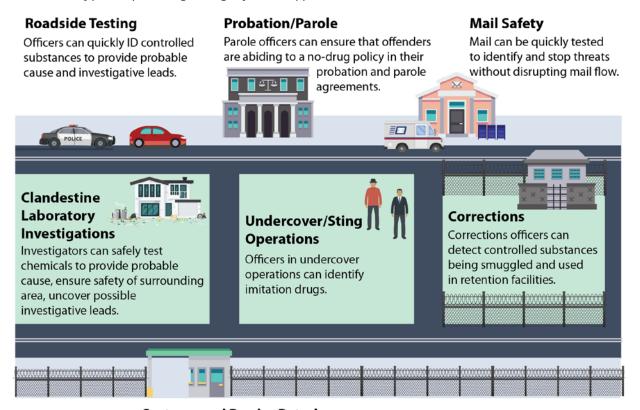
Introduction

Illegal use and circulation of controlled substances constitute a significant public safety issue in the United States. As a result, an individual found to synthesize, possess, and distribute drugs regulated into one of five schedules (or analogous to these scheduled compounds) can face substantial jail time and fines, depending upon the compositions and amounts of the substances in their possession [3]. Many law enforcement and government agencies use presumptive tests as a means for a reasonable search and seizure. Presumptive drug testing often occurs in a field setting, such as on the roadside during a traffic stop. In recent years, procedures surrounding how to conduct presumptive drug tests have become increasingly important to ensure the safety of law enforcement personnel, as some of the substances tested pose safety hazards to those identifying unknown chemicals in the field. [4-6]

Purpose of Presumptive Drug Testing

The goal of presumptive drug testing in the field is to provide a preliminary result suggesting the presence of specific drugs or unknown substances (e.g., adulterants). The role of presumptive drug testing heavily depends on a jurisdiction's regulations and policies, different subsets of which may apply to different agencies. **Exhibit 1** depicts the role of presumptive drug testing in forensic applications.

Exhibit 1. The role of presumptive drug testing in forensic applications



Customs and Border Patrol

Border patrol can quickly identify dangerous and controlled substances to seize and prevent further transport inside the borders.

Technologies Used for Presumptive Drug Testing

Presumptive drug testing in the field started with, and has largely remained dominated by, color-based testing [7]. These tests use chemical reactions and an associated color change to tentatively identify a drug or drug class. While these tests have provided value to law enforcement agencies for decades, they have limitations:

- Color-based tests are not always effective with newly synthesized drugs because they do not identify the chemical
 structure; instead, these tests only detect the presence of specific functional groups [8]. For example, the DuquenoisLevine reagent in a test for marijuana reacts with the free para position on the phenol group of molecules with long
 aliphatic tails, such as tetrahydrocannabinol (THC). Most synthetic cannabinoids do not possess these functional groups.
- The influx of novel psychoactive substances has challenged the utility of inexpensive, single-use tests, as not all
 presumptive tests for traditional drugs react to these new substances. These tests may also indicate false positives and
 false negatives.
- Color-based tests are not always accurate, a limitation that has led to public scrutiny of these tests.

More recently, technologies typically confined to the laboratory have been adapted for use in the field, offering a level of analysis far beyond that of traditional color-based testing. Manufacturers have engineered laboratory instruments, such as Raman spectrometers and mass spectrometers, to be rugged and field-portable. These technologies are more adaptable than color-based tests because they analyze the chemical structures of unknown substances, which positions them as useful instrumentation for substance identification in the field.

In essence, a color-based test answers the question "is this substance likely cocaine?", whereas portable laboratory instrumentation answers the question "what is this substance?"

This report provides a landscape view of these newer handheld and portable field drug testing technologies, including ion mobility spectrometry (IMS), mass spectrometry (MS), infrared spectroscopy (IR), and Raman spectroscopy as highlighted in **Exhibit 2**. Other technologies, such as fluorescence and thin-layer chromatography (TLC) are not discussed in detail in this report because of their current limited utility and commercial availability in field-portable form. Additional emerging field testing technologies are discussed on page 33.

Exhibit 2. Highlights of technologies used for presumptive drug testing in the field

Technology	Identification based on	Benefits	More Information
Mass Spectrometry (MS)	Molecular weight and chemical structure	Robust	Page 21
Ion Mobility Spectrometry (IMS)	Molecular size and shape	Extremely sensitive	Page 22
Raman Spectroscopy (Raman)	Chemical structure	Able to scan through some packaging	Page 23
Infrared Spectroscopy (IR)	Chemical structure	Highly selective	Page 24

Implementing Portable Presumptive Field Testing Devices

Law enforcement agencies, armed forces, and other users of presumptive drug testing must carefully consider the available options before purchasing and implementing a portable drug testing device. Although each type of instrument possesses unique qualities, the general benefits and challenges of these types of instruments include the following:

Potential Benefits

- Instrument versatility—Depending on the size on their onboard spectral library, these portable drug testing devices can identify a large number of unknown substances, including adulterants, diluents, and drug precursors in one test. The comprehensive nature of these devices eliminates the need to carry multiple, single-indication tests and choose which types to use, which saves time and increases the chances of presumptively identifying a substance. Agencies using these devices can conduct basically an unlimited number of tests, unlike officers using color-based tests, which are priced per test. Thus, resources do not limit the amount of presumptive testing conducted on-site.
- **Objectivity**—Whereas the interpretation of color-based tests depends on the visual acuity of the test administrator, many portable instruments provide a non-ambiguous test result. Such devices can identify the compound(s) present or function as a "red light, green light system," notifying the user when a controlled substance is detected. These features reduce the risk of misinterpreting results at the scene.
- **Specificity**—Portable presumptive drug testing devices are less prone to false negatives and false positives than single-use, color-based tests. As a result, law enforcement can feel more confident that these tests are correctly identifying controlled substances.
- Safety—Some portable presumptive drug testing devices, such as Raman spectrometers, allow the user to scan through clear packaging. Many others are sensitive enough to detect drugs on samples taken from the exterior of packaging. These capabilities can reduce exposure to an unknown substance.
- Chain of custody corroboration—Many of these portable units store time-stamped test results on the device and can easily export spectra and chemical identification results to a computer for further analysis. In contrast, the results of color-based tests are difficult to document and degrade over time. Detailed test records can facilitate the defense of presumptive tests in court.
- **Technical support**—Many device manufacturers offer technical support, which allows users to send results to experts for assistance with interpretation. These experts are an important resource for troubleshooting. In addition, some agencies may choose to use chemists in the forensic labs as resources to help interpret test results, depending on their resources.
- Multiple applications—Portable field testing devices can provide value not only for law enforcement applications focusing
 on presumptive drug testing but also for other chemical identification roles in the field and laboratory. These devices'
 versatile applications can help justify their high up-front costs and may enable cost sharing between different units of an
 agency or between law enforcement agencies in the same location. Exhibit 3 describes possible applications of these
 portable devices outside of presumptive drug identification.

Exhibit 3. Potential applications of portable presumptive drug testing devices

Application	Use for Portable Device					
Law enforcement/first responders	Safety and risk mitigation on scene					
Forensic laboratory	Preliminary testing					
Hazardous materials (hazmat)	Rapid identification of unknown chemicals in a field setting					
Military	Chemical warfare agent (CWA) defense					
Transportation Safety Administration (TSA)	Drug and explosive detection in airports					

Potential Challenges

- **High up-front cost**—Purchasing a portable drug testing device can be a significant up-front expense for many agencies. Some manufacturers offer lower-cost leasing options.
- Complexity—Although many of these instruments are designed to be used by individuals without a background in chemical analysis, some require training to accurately perform tests and troubleshooting. Some instruments, such as gas chromatography (GC)-MS, require more training to operate. Quality assurance procedures are critical for demonstrating reliable results, and require procedures, such as running blanks before testing substances. Some agencies may be reluctant to adopt these technologies based on their perceived complexity to use.
- Maintenance—Unlike traditional color-based tests that are single use, these portable instruments are used repeatedly and
 must be checked periodically; for example, regularly updating the instrument's software is critical for reliably detecting
 new drugs that are increasingly popular and frequently encountered in the field.
- Limited mixture interpretation—Interpreting mixtures of drugs remains a significant challenge for most presumptive drug tests, and portable instruments are no exception. For some instruments, the presence of certain substances, such as acetaminophen, in mixtures may mask the presence of other components. Mixtures containing components in very small proportions (<1%) are also particularly problematic and may lead to false-negative readings (e.g., fentanyl).
- Library dependence—Many portable field testing instruments are dependent on an up-to-date library. It is important that the instrument's library can receive updates or be user-customizable because new drugs and novel psychoactive substances (NPSs) are hitting the streets every day. If agencies are using an out-of-date library or a library that has not been validated, new substances that may pose a threat will not be identifiable. Instrument operators must factor in the comprehensiveness and limitations of the library to make appropriate decisions on the test results.

Economics of Instruments vs. Single-use, Color-based Tests

Portable presumptive drug testing instruments and single-use, color-based tests have comparable costs over time, despite the large up-front price difference.

Single-use, Color-based Tests:

Color-based tests typically cost a few dollars (\$2–5) per test. A law enforcement agency based in a large metropolitan area may make approximately 5,000 drug-related arrests per year, and two color-based tests are likely used per arrest. Assuming an average cost of \$3/test, the resulting cost would be roughly \$30,000 per year for that jurisdiction.

Instruments:

The average price ranges of portable instruments depend on the technology:

MS: \$50,000 +
GC-MS: \$50,000 +
IMS: \$25,000-\$37,500
Raman: \$12,500-\$25,000

IR: \$25,000-\$37,500

Keep in mind there may be yearly consumables costs (e.g., sample collection materials, gas canisters) associated with certain technologies. These typically average to less than \$1/test.

Because portable field testing instrumentation can be used for multiple years, the total cost of these instruments may be quite comparable to the total cost of color-based tests.

Choosing the Right Presumptive Portable Field Testing Instrument

The available field testing technologies each have their own strengths and weaknesses, and no single device will suit the needs of all jurisdictions. Agencies looking to implement a portable field testing instrument to expand beyond color-based testing should consider application-specific factors related to the intended application and the specific circumstances of the agency.

Summary of Available Presumptive Drug Testing Technologies

Exhibit 4 provides an overview of available technologies for presumptive testing and some important considerations for purchasing and implementing these devices in the field.

Application-Specific Factors

- Amount of sample present—Different types of devices are suited to different volumes of suspected drugs encountered in the field. Raman and IR technologies require a visible quantity of the substance to be analyzed for an accurate reading, which may be appropriate for typical roadside drug testing and clandestine laboratory applications. In contrast, IMS and MS are particularly sensitive and can easily detect trace amounts not visible to the naked eye collected via swab from the exterior of a package or other surface. Thus, IMS and MS may prove useful for applications such as mail safety and in circumstances where it is advantageous for a user to not have to open the packaging and risk exposure to dangerous substances, such as fentanyl.
- **Drug packaging**—Raman devices are highly useful in areas where drugs are typically packaged in clear plastic bags but less so in areas where law enforcement officers frequently encounter substances contained in wax paper, aluminum foil, or dark vials. For example, agencies in Pittsburgh, Pennsylvania, factored in the prevalence of non-translucent heroin packaging when choosing potential portable presumptive drug testing devices (see more on page 16).
- Phase of unknown sample—Different phases of unknown substances are encountered in different field applications of
 drug testing devices. For example, law enforcement officers performing roadside drug tests may primarily handle solid
 powders, whereas those investigating clandestine labs may also encounter unknown liquids and vapors. MS-based systems
 are the most versatile. Most devices can adequately sample solids and liquids, but MS systems are best suited to detecting
 vapors.
- Commonality of emerging drugs—Field testing devices often rely on an onboard library to identify unknown substances. Unless the user is trained in interpretation, such devices can only identify what is contained in their libraries. Agencies that frequently encounter newly emerging drugs, such as NPSs, should strongly consider a device with frequent library updates or the ability to add reference spectra.
- Time available for analysis—The start-up time and time between each test vary between devices. Quicker testing methods often have a tradeoff, such as higher cost or lower sensitivity or specificity. Agencies that perform high-throughput testing (e.g., mail safety) or whose staff must hold a suspect during the drug identification process would likely benefit from faster devices.
- Location of use—Users who perform presumptive drug testing in multiple locations will likely store the testing devices in their cars. Thus, those agencies should consider purchasing smaller devices that have long battery lives and can tolerate extreme temperatures. In contrast, personnel working at more permanent setups in satellite testing locations may prefer larger units with AC power.

Exhibit 4. Properties of field portable devices for presumptive drug testing

		Costs		User Expe	rience				Device Performa	nce			
	Average up-front cost (S)*	Typical consumables cost per test	Typical protection from substance ¹	Typical ease of use ²	Typical portability ³	Point and shoot	Minimum sample required (relative)	Approximate startup and test times (scale in minutes)	Not prone to overload from excess sample	Non- destructive sampling	Tests solids	Tests liquids	Tests vapors
MS	\$\$\$\$\$	< \$1 model dependent	2 3	2 3	2 3	-		0 15 30 45 startup time: 5–7 min test time: 10–30 sec	-	-	model dependent	model dependent	model dependent
GC-MS	\$\$\$\$\$	\$1 model dependent	2 3	2 3	2 3	-		0 15 30 45 startup time: 5–30 min test time: 4–15 min	-	-	model dependent	√	✓
IMS	\$\$\$ \$\$	<\$1	2 3	2 3	2 3	model dependent		0 15 30 45 startup time: 15–30 min test time: 10–30 sec	-	-	√	√	✓
Raman	\$\$ \$\$\$	\$0	2 3	2 3	2 3	✓		0 15 30 45 startup time: 1 min test time: 1-2 min	√	√	√	√	-
IR	\$\$\$ \$\$	\$0	1 3 4	1 2 3	1 2 3	model dependent		IR (benchtop portable) 0 15 30 45 startup time: 30 min test time: 1 min IR (handheld) startup time: 10 min test time: 2 min	√	√	√	✓	-
Color- based	N/A	\$2–\$5 per test	2 3	2 3	2 3	-		0 15 30 45 startup time: 0 min test time: 2 min	√	-	√	√	-

* Price Scale

Protection from Substance 1—
Sample removed and manipulated 2—
Sample removed and analyzed as is
A-Package opened but no sample removed 4—
Sample through packaging

² Ease of Use

- 1—Operation and interpretation requires technical sophistication
- 2—Operation and interpretation requires significant training 3—Simple to operate, difficult to interpret
- 4—Simple to operate and interpret

³ Portability

- 1—Larger portable instrument that typically relies on AC power
- 2—Mid-size portable instrument that typically relies on battery power 3— Small handheld portable instrument that typically relies on battery power 4— Requires no power

Agency- and Jurisdiction-specific Factors

- **Size of the jurisdiction**—Agencies serving smaller physical areas may have less need for presumptive testing and may be able to consider a field testing setup in which multiple personnel use a single device located at a central facility.
- Agency budget—Portable presumptive field drug testing devices vary widely in price, as shown in Exhibit 4. Agencies may
 need to factor in the number of devices they need to purchase in the decision-making process.
- Laboratory support—Because portable drug testing instruments are developed from technologically sophisticated laboratory instrumentation, their outputs may require further data interpretation. Agencies without resources such as scientists in an affiliated forensic laboratory may prefer to purchase devices from a manufacturer that provides on-demand data interpretation services.
- **Future use of data**—In many circumstances, presumptive test results could be used later in drug investigations. Agencies should consider how instruments store and output data, and accessories to these devices, such as computers, tablets, and printers. For example, if results need to be stored individually with the rest of the documentation for a specific case, a system that generates pdf reports would be more fitting than a system that only stores raw spectra or data in a format only readable by the instrument software.
- Personnel safety—Devices that are capable of analyzing through containers or are sensitive enough to sample from the
 exterior of packaging offer additional personnel safety. Depending on agency protocols, these added safety measures may
 be more or less valuable. For example, if testing is performed while wearing significant protective gear, such as a hazmat
 suit, the added specificity and sensitivity of MS may be more valuable than the ability of Raman to sample through a
 container.
- Time available for training—Some technologies, such as MS, require more extensive training and periodic re-training than others, such as IR and Raman. If an agency does not have the resources to invest in up-front and refresher training, it would be prudent to invest in devices with streamlined interfaces that guide user input.

Use Profiles

Multiple law enforcement agencies are using portable presumptive drug testing devices in the field, whether for the presumptive identification of drugs or similar chemical identification applications. The following profiles capture insights from four different agencies who selected, purchased, and implemented devices in field settings:

- Raman—Roadside testing, Lt. Patrick Glynn, Quincy Police Department
- MS, GC-MS—Military and first responder chemical identification, Dr. Phillip Mach, Edgewood Chemical Biological Center (ECBC)
- GC-MS, Raman, IR—Hazmat teams, David Matthew, Deputy Chief (ret.) Kansas and California Fire Services
- IMS—Overdose Task Forces (OTFs), Josh Yohannan, Allegheny County Office of the Medical Examiner

Use of Raman: TruNarc™ handheld narcotics analyzer used by the Quincy, Massachusetts Police Department

Lieutenant Detective Patrick Glynn serves as the Commander of the Special Investigations and Narcotics Units of the Quincy Police Department.

The Drug Control Unit of the Quincy Police Department uses the TruNarc Handheld Narcotics Analyzer for presumptive drug testing in the field. The Quincy Police Department has access to three TruNarc instruments: (1) The **drug unit** has an instrument available at all times when they are in the field. (2) **Patrol officers** have access to a unit on an as-needed basis. (3) **Booking area staff** have access to a unit if substances that were initially missed are discovered during the booking process; this unit is also made available to other officers on the force.

Prior to procuring a TruNarc a few years ago, the Quincy Police Department used color-based tests for field testing. For this department, incorporating the TruNarc into their presumptive drug testing routine has been straightforward. They find the device's **portability** to be convenient, and the only performance issues they have encountered are related to **battery life**. Additionally, they have found that the **onboard reference library** is updated frequently enough to satisfy their needs as an agency that often encounters NPSs, and the process by which ThermoFisher provides updates to their instrument software is convenient. Lt. Glynn mentioned three main advantages of this relatively sophisticated instrument:

- 1. **Speed:** The use of the TruNarc has significantly decreased the amount of time that presumptive testing takes in the field. Lt. Glynn mentioned that previously, presumptive tests were very time consuming because each test was specific to a certain type of drug, and multiple tests had to be used to test one substance. With the TruNarc, officers only have to scan a substance once for a tentative identification.
- 2. Accuracy: Lt. Glynn noted that the TruNarc is more accurate than presumptive color-based tests because it can **better distinguish** between drug analogs in fewer steps and **less time** than traditional color-based tests. Officers are more confident in their results using the TruNarc than they were with color-based tests.
- 3. **Safety:** For the Quincy Police Department, safety is the greatest advantage to using the TruNarc over color-based tests, and it is one of the main reasons that they made the switch to using portable Raman. Unlike color-based tests that require officers to remove dangerous substances from packaging, often multiple times, testing with the TruNarc requires minimal or no officer contact with the substance in question. He mentioned that with the rise in popularity of synthetic opioids, such as fentanyl, this type of device is incredibly valuable. Indeed, Lt. Glynn noted that increased safety alone practically justifies the cost of the instrument.

"TruNarc is a great tool and has been really beneficial to us and the officers."

"Utilizing the TruNarc is like bringing the lab to the street. The TruNarc is not a luxury but a necessity!"

-Lieutenant Detective Patrick Glynn

All Quincy Police Department officers who use the instrument are trained prior to field use and undergo annual refresher training. Initial user training consists of a 4-hour lecture and hands-on experience with the instrument. Training is conducted by one of the officers in the drug unit who also trains personnel from other agencies. Lt. Glynn mentioned that patrol officers and investigators only use the instrument when they are in the presence of a member of the drug control unit. Additionally, the department has trained defense attorneys in their jurisdiction on the technology, and thus, the attorneys are better able to advise clients based on their knowledge of the instrument and its reliability.

Device Benefits:

- Quick, accurate, and safe compared to traditional presumptive drug tests
- Very convenient: portable instrument with library updates every 3-6 months

Lessons Learned:

- Battery life may cause issues during extended use in the field—multiple batteries can be purchased and interchanged as necessary to combat this issue
- TruNarc training for defense attorneys has reduced some of the challenges faced in the courtroom

Use of MS: The U.S. Army Edgewood Chemical Biological Center evaluation of mini mass spectrometers for chemical identification applications for military personnel and first responders

Dr. Phillip Mach is a researcher at the ECBC, located within the Aberdeen Proving Ground, Aberdeen, Maryland.

The ECBC specializes in non-medical chemical and biological defense research and technology development. Research topics at this institution are strongly connected to chemical identification, such as diagnostics for individuals affected by chemical warfare agents (CWAs), detection of trace quantities of chemicals, and chemical decontamination methods.

The ECBC is home to a BioDefense Mass Spectrometry Core Facility and a Portable Mass Spectrometry test site that house approximately a dozen models and brands of miniaturized, portable mass spectrometers. The facility was developed to assist defense agencies in choosing the right portable mass spectrometer for their needs. This division of the ECBC tests various equipment, helps customize instrumentation for defense operations, offers guidance on the needs for developing future generations of equipment, and helps agencies within the Department of Defense and Department of Homeland Security convey the value of these instruments to decision makers. In addition, personnel at the ECBC organize trainings for soldiers and subject matter experts, focusing on instrument operation, maintenance, and hands-on experience through mock field trials. Although this center does not focus specifically on forensic science applications, it does serve agencies using or considering implementing portable MS for chemical and biological identification applications in the field.

Dr. Phillip Mach and his colleagues have studied a wide array of analytes using these devices, including CWAs, their hydrolysis products, and toxic industrial chemicals. Dr. Mach explained that these instruments can also be used in the field to conduct presumptive tests for opioids, which are often problematic to the forensic community because of their high potency and low concentrations in samples.

Currently, commercially available mini mass spectrometers vary widely in terms of their capabilities and qualities. Dr. Mach provided insight into important instrument characteristics that agencies must consider when purchasing and implementing mini MS technology for presumptive drug testing purposes:

- Sample introduction methods—Some portable MS units can introduce samples in the vapor, liquid, and gas phases, whereas others are only capable of sample introduction in one of these phases. End users should be aware of the types of samples that they plan to analyze and the method of introduction required (i.e., does the drug need to be dissolved before introduction, and is this feasible?). Some sample introduction methods may be simpler to perform for a non-expert, leading to time savings in the field. For example, instruments that allow for solid-phase microextraction (SPME) introduction, such as the Smith's Detection GUARDION™ portable GC-MS, may require little to no sample prep. Furthermore, some methods, including SPME, may allow for "fetch and retrieve" sample collection. Personnel in the field could set up the instrument at the field site while collecting samples through a pen containing the SPME fiber for analysis. Thus, personnel only need to carry a small SPME collection device instead of the entire instrument.
- **Self-contained units**—Self-contained units are typically **easier to transport** and do not require a large external carrier gas cylinder or roughing pump. Users can easily transport the unit to and from a scene and move it around as necessary.
- Frequency of library updates—Up-to-date libraries are critical to identifying an unknown substance at a scene; end users should ensure that the instrument of choice has a library that is kept up-to-date by the manufacturer. Although many well-known reference libraries (e.g., NIST and SWGDRUG) are compatible with most MS instruments, different libraries are needed for different ionization sources.
- Chromatographic Temperature—Not all GC-MS instruments can analyze certain substances, such as fentanyl, because their GC columns may not be capable of sufficient vaporization temperatures. If a sample is introduced that the temperature is not high enough to vaporize, the instrument may become compromised until it is serviced by the manufacturer. When searching for an instrument to purchase, it is important to ensure that the unit contains a column compatible with expected vaporization temperatures, and that the temperature ramps high enough to elute (remove from the column) commonly encountered unknowns in the field. The BaySpec Portability™ and Smiths Detection GUARDION™ are examples of instruments that can analyze fentanyl and its analogs in the field.

Dr. Mach also noted that despite rapid technology advancement in recent years, portable MS systems still possess limitations in the field. It is critical that these instruments be ruggedized and shockproof for transportation and field work, but many MS instruments tested in the ECBC facility are not. Furthermore, although these instruments have been adapted for use by non-experts, such as first responders, Dr. Mach noted that without a fully developed library, some of these instruments may not be useful for an individual without a scientific background.

Device Benefits:

- Time savings through improved sampling methods: the use of advanced sample introduction methods, such as SPME, in MS instruments facilitates quick sample introduction with little to no preparation and, thereby, quick and easy analysis in the field.
- MS is a technique that typically works well for the analysis of trace amounts of substances and mixtures.

Lessons Learned:

- Shockproof and ruggedized features are important for a mini mass spectrometer to be "field-proof."
- Not all mini mass spectrometers can analyze certain substances, such as fentanyl. This limitation could cause issues in the field when the instrument operator is confronted with an unknown substance.
- Sample introduction methods can influence how simple an instrument is to operate for a non-expert.

The conclusions expressed here by Dr. Mach are not the official policy of the U.S. Army, ECBC, or the U.S. government.

Use of a variety of portable technologies, including Raman, IR, and GC-MS, by hazmat teams

David Matthew, M.A. is a 30-year veteran of the public safety field, working primarily in Kansas and California. He serves as a consultant and subject matter expert in public safety issues at the local, state, and federal levels. His experience with handheld chemical identification devices relates to hazmat response teams.

Hazmat response teams need to identify unknown compounds quickly to make risk-based decisions. Being able to quickly determine whether a threat is credible enables them to ensure public safety and limit unnecessary panic.

Matthew sees many parallels between hazmat chemical identification and presumptive drug testing in the field, especially in regard to clandestine laboratory investigations. For chemical identification purposes, hazmat teams use the same types of portable analytical instruments that are used for field testing of drugs, including portable Raman, Fourier transform IR (FTIR), and GC-MS technologies. Both hazmat and presumptive drug testing users need portable devices to obtain rapid results that allow them to efficiently address the situation at hand. Similar to many officers performing field drug tests, hazmat responders are trained to collect data but not necessarily to interpret the data. For this reason, technical interpretation support is important. Matthew values different chemical detectors for specific reasons:

"Our responders are trained to get good data, not necessarily to interpret the data. Portable instrumentation such as Raman, IR, and GC-MS allows us to obtain good data and make more effective risk-based decisions."

—David Matthew

- Raman is a **non-destructive method** that supports chain of custody through its ability to sample within a vial that can be stored for further analysis.
- Attenuated total reflection (ATR-FTIR), which makes direct contact with the unknown sample, gives results that are reliable and **reproducible** in the field and the laboratory.
- GC-MS is able to identify unknown gases and vapors with high confidence using complex separation methods. Sampling techniques utilizing SPME fibers have proven effective in GC-MS identification of volatile organic compounds in low concentrations (e.g., to identify trace amounts of accelerants during a fire investigation).

These portable technologies possess features useful for general law enforcement applications, clandestine laboratory investigations, and hazmat applications. **Exhibit 5** demonstrates some of the similarities and differences between these applications.

Exhibit 5. Differences between hazmat and law enforcement use of portable Raman, IR, and GC-MS technologies

Difference	Law Enforcement Applications	Hazmat and Clandestine Laboratory Applications	Comments					
Commonly encountered substances	Solids (e.g., white powders)	Solids, liquids, and gases	GC-MS can analyze solids, liquids, and gases. It is the instrument of choice for vapors because of the ease of collecting and analyzing gases using this technique.					
Processing a scene	Typically use one instrument for presumptive drug testing at a scene	Use multiple instruments and/or techniques to process a single scene	The use of multiple devices increases the confidence that an unknown substance has been accurately identified. It is critical that hazmat personnel accurately identify substances for public safety purposes. In contrast, although accurate identification is important to law enforcement, officers typically perform presumptive tests, and thus, just one instrument is usually needed.					

Difference	Law Enforcement Applications	Hazmat and Clandestine Laboratory Applications	Comments
Personal protective equipment (PPE)	Gloves	Specially designed suits and self-contained breathing apparatuses	PPE provides safety, and thus, minimal exposure during sampling may be a lower priority for hazmat teams than speed and accuracy. Hazmat personnel may also prioritize devices that are easy to operate while wearing PPE.
Sample environment	Usually inside a container or other packaging	Uncontained	Because of their use of specifically designed PPE, hazmat personnel are typically less concerned with being able to sample through a container.

Lessons Learned:

- Commercially available, portable technologies are simple to operate. Users without an analytical chemistry background can successfully use these devices.
- Portable instrumentation provides real-time information to help personnel make better-informed decisions in the field.

Overdose task forces in Pennsylvania considering the Bruker Roadrunner IMS device for presumptive drug testing in the field

Joshua Yohannan serves as drug chemistry laboratory manager for the trace and drug chemistry sections of the Allegheny County Medical Examiner's Office, which supports law enforcement as a fully functional drug chemistry forensic laboratory. He oversees the analysis of samples related to over 6,000 cases involving suspected controlled substances per year.

Most law enforcement agencies in Pennsylvania have halted presumptive field testing because of safety concerns around fentanyl. When officers encounter suspected controlled substances, they are instructed to send samples to the laboratory for identification without testing them in the field, ultimately increasing the number of samples being submitted for analysis. This increase has overwhelmed some laboratories, who must focus primarily on cases requested for court because cases in the federal system cannot go to grand jury without confirmatory results. Overwhelming caseloads in Pennsylvania have led to the establishment of the overdose task forces (OTFs), a group consisting of law enforcement, medical professionals, and legal representatives. One OTF responsibility is recommending portable presumptive drug testing devices that could relieve the increased pressure on laboratories.

Some OTFs in Pennsylvania are considering using the Roadrunner IMS system for presumptive drug testing in the field.

Yohannan identified IMS as a possible suitable presumptive testing device based on a news article from NIST [9]. IMS can detect substances present at very low levels. Thus, test administrators can swab the external packaging to obtain results without increasing their risk of exposure by opening the packaging. He found the Bruker Roadrunner instrument to be well adapted to the field as a lightweight, battery-powered device that is effective at detecting fentanyl and its analogs in low concentrations. The Roadrunner uses a non-radioactive ionization source, which is safe for officers to operate. Although he appreciates the high sensitivity of the device, Yohannan noted that users may encounter issues with overloading the instrument. If a sample overloads the instrument, it can take approximately 20 minutes to clear the system and ready the instrument for further use. As for most technologies, drug mixtures can affect the results, and Yohannan has seen instances

"IMS allows the law enforcement officer to identify an unknown compound just by swabbing around the package, eliminating the need to open the packaging. The Overdose Task Forces are seriously considering use of this technology in the field."

—Joshua Yohannan

where heroin and fentanyl are indistinguishable using this instrument. However, future library updates may facilitate identification. For example, the RoadRunner could identify and differentiate cyclopropyl fentanyl and methoxyacetyl fentanyl after these substances were added to its library.

Yohannan explained that some agencies in Pennsylvania have employed portable Raman devices in the field, which are capable of scanning through clear packaging materials. This type of technology is beneficial, as it increases the safety of law enforcement personnel by negating the need to open the packaging to presumptively identify the substance. In Pittsburgh, however, this benefit is limited, as most heroin samples (the most commonly encountered controlled substance in the Pittsburgh area) are contained in opaque wax packaging. Unlike Raman, the sensitivity of IMS technology may enable safe sampling procedures with this type of packaging.

Device Benefits:

- Safe sampling: using these devices often avoids the need to open packages because of their sensitivity.
- Portability: using a lightweight device with battery power facilitates analyses in multiple types of field settings.

Lessons Learned:

- Sensitivity is both a benefit and a challenge to users, as too much sensitivity can cause processing delays. Proper training and sampling is required for users.
- When choosing the most appropriate device, agencies must consider specific circumstances of their jurisdiction, such as common types of drugs and packaging materials.

Factors Affecting Presumptive Drug Testing in the Field

Although law enforcement agencies have been using presumptive drug tests in the field for decades, several factors have affected how agencies have used these tests, including NPSs, drug mixtures, and user safety.

Novel Psychoactive Substances

NPSs, a term adopted by the United Nation's Commission on Narcotic Drugs in 2012, are typically synthetic compounds that produce effects similar to those of traditional drugs, such as opioids, cathinones, and cannabinoids [10]. Production and purchase of most NPSs are not specifically prohibited, before legislation is modified and these compounds are specifically designated as scheduled substances. Many NPSs have been slightly altered from compounds such as pharmaceutical products or laboratory-synthesized therapeutic drugs by clandestine chemists who capitalize on readily-accessible scientific literature and patents. Although NPSs have been circulating within the drug market since the introduction of the synthetic drug 3,4-methylenedioxymethamphetamine (MDMA) in the 1980s, the number of unique chemical formulations circulating has increased almost exponentially. The United Nations Office for Drugs and Crime reported that 644 NPSs were identified by 102 countries in 2008–2015 [11]. This new and rapidly expanding class of drugs has presented multiple challenges for presumptive testing in the field, as described below:

Identification

The rapidly increasing rate of unique NPSs entering the drug market has proven to be a significant challenge for presumptive drug testing. Manufacturers of color-based drug tests, whose presumptive test kits are designed to detect the presence of one or a limited number of drugs, cannot keep up with the rate of new drugs being developed. In addition, law enforcement agencies do not have the budget or space to store countless expirable, single-use tests specific to each drug type. Although color-based tests for certain types of NPSs are sold, the varieties that are currently available cannot detect a wide range of drugs and may lead to false-negative results. For example, multiple manufacturers sell color-based tests to identify synthetic cathinones, often referred to as "bath salts"; however, more than 100 types of cathinones have been identified, making color-based tests insufficient [12].

Portable presumptive drug testing instruments can be an effective solution to identifying NPSs by comparing spectra generated from analyzing an unknown compound against a library of known compounds. While developing and implementing color tests for new NPSs may take a year or more to develop, a simple software update can allow an instrument to detect the new device. Depending on the model used, these portable devices can store thousands of discrete spectra from thousands of different compounds.

Regulation

Regulations on NPSs also represent a complicating factor in interdiction efforts. Despite multiple rounds of legislation passed by the Drug Enforcement Administration (DEA) to control the use of these compounds, regulations are difficult to enforce. For example, the Controlled Substances Analogue Enforcement Act of 1986 considers analogs of controlled substances, such as NPSs, to be controlled substances if they are intended for human consumption. Thus, many NPSs are packaged with the phrasing "not intended for human consumption" to circumvent this regulation. Furthermore, although the legislation essentially treats analogs of Schedule I controlled substances as Schedule I drugs, what is truly considered an analog of one of these drugs is subjective. For example, in some cases, NPSs may mimic the effects of scheduled drugs, such as cannabis or methamphetamine, but have dissimilar chemical structures [13]. Passing and enforcing legislation that controls the creation and sale of NPSs while still allowing the development of novel therapeutic compounds is challenging. In fact, many NPSs were derived from therapeutic compounds developed in a laboratory. For example, one measure undertaken to convict traffickers of possessing NPSs is the DEA's temporary scheduling of all structural variants of fentanyl. This legislation is intended to control synthesis and distribution of harmful drugs, but it also affects any therapeutic compounds that are structural variants of fentanyl.

Recent United States Legislation Concerning Novel Psychoactive Substances

2011: Attorney General temporarily lists eight NPSs (five synthetic cannabinoids and three synthetic cathinones) on Schedule I of the Controlled Substances Act (CSA) [14, 15].

2012: The Synthetic Drug Abuse Prevention Act, an amendment to the CSA that places 26 substances (synthetic cannabinoids, stimulants, and hallucinogens) in Schedule I, is enacted [16].

2013–2015: The DEA places 10 synthetic cannabinoids, three synthetic phenethylamines, 10 synthetic cathinones, and the opioid acetyl fentanyl on Schedule I [17].

2016-2018: 50+ NPSs were listed as Schedule I substances [18].

2018: Placement of all fentanyl structural variants on schedule on an emergency basis [19].

Emerging Substance Knowledge

NPSs also pose a challenge to law enforcement because they are, as illustrated by their name, new compounds. Although both scientists and law enforcement have developed extensive knowledge of the intricacies of traditional drugs, such as methamphetamine, heroin, and cocaine, very little research has addressed these new NPSs and their effects. Lack of experience with NPSs and the sheer number of unique compounds circulating make it difficult for law enforcement (and emergency responders) to recognize these drugs and their adverse effects in users. Many of these synthetic compounds are extremely dangerous if ingested and may be fatal, even in small amounts. Law enforcement personnel assume a significant amount of risk when they investigate unknown powders in the field. Continued research on the landscape of NPSs and increased training for law enforcement to better recognize and react to NPSs during drug interdiction efforts and overdose responses will increase the confidence of law enforcement in the field.

Understanding Novel Psychoactive Substances

In the past few years, toxicologists and analytical chemists have been actively researching the effects of popular NPSs in the United States. Helpful reviews of this new drug class include the following:

Reports of Adverse Effects Associated with Use of Novel Psychoactive Substances, 2013–2016: A Review [20]

Graphic Overview of NPS Types [21]

Drug Mixtures

Law enforcement officers primarily encounter traditional illicit drugs, such as cocaine, methamphetamine, and heroin. However, these drugs are not always found in their pure form. A recent study in the United Kingdom reported that out of 500 samples of cocaine tested, cocaine was the sole active ingredient in only 10% [22]. Diluents and cutting agents are incorporated to add bulk and increase the sellable weight. Additional adulterants are added to drugs to enhance or alter their effects and can be readily available prescription drugs or other illicit drugs. For example, the anesthetic benzocaine is commonly used as a cutting agent for cocaine [23].

Drug mixtures, especially those containing adulterants, pose a significant challenge for presumptive testing in the field. Color-based tests are usually not designed to identify adulterants commonly used in illicit drugs or may fail to detect an adulterant if it is added in a low concentration. Furthermore, when dangerous adulterants, such as fentanyl, are added to drugs, they pose a risk to law enforcement. Although relatively sophisticated field technologies, such as Raman and FTIR, may be able to identify diluents and adulterants in a sample (depending on the contents of their onboard libraries), these devices sometimes struggle to interpret drug mixtures. For example, certain types of cutting agents, such as acetaminophen, can mask illicit drugs or make it difficult to make an accurate identification. Technologies that incorporate a separation step before characterization, such as GC-MS, could address the challenge of mixtures in presumptive field drug analysis. More information on GC-MS can be found on page 21, and additional research on future technologies can be found on page 33.

User Safety

The rise of NPSs and drug mixtures has brought concerns of user safety to light. Users of color-based presumptive drug tests must directly handle unknown substances by opening containers and often transferring powders to the test kits for analysis, which may cause these substances to aerosolize. Thus, law enforcement personnel may ingest these drugs through inhalation or skin absorption. Although many drugs pose a threat to officers who accidentally ingest them while conducting presumptive drug tests, the primary subject of this concern is the possibility of officer overdoses related to handling fentanyl or other synthetic opioids. For example, an Ohio police officer overdosed from fentanyl exposure in a vehicle while responding to a traffic stop and required four doses of Narcan [25].

Safety is a major concern for individuals conducting presumptive tests in the field, regardless of the type of test being used. Methods that can help to improve user safety include the following:

- Investing in technologies that scan through a container (Raman).
- Purchasing technologies that can detect trace amounts of substances, including on the exterior of a package (IMS).
- Providing specific training on assessing unknown substances during drug interdiction efforts.
- Advocating increased use of personal protective equipment (PPE), such as air purifying respirators or selfcontained breathing apparatuses during drug investigations [26].
- Deploying forensic laboratory chemists to the field to test unknown substances.

Fentanyl

Used as an analgesic for chronic pain in cancer patients, this opioid is up to 50 times more potent than heroin, and certain analogs, called "fentalogues," can kill an adult who ingests as little as 2-3 milligrams of the substance. Today, a significant percentage of drug overdoses and deaths in the United States is related to fentanyl. For example, in New York City, in 2016, 44% of overdoserelated deaths stemmed from fentanyl ingestion [24]. Fentanyl is often incorporated into heroin but can be found in a variety of drug mixtures: in 2017, the New York City Police Department laboratory reported seizures of cocaine, counterfeit prescription pills, methamphetamine, and ketamine laced with fentanyl [24]. The DEA has identified more than 15 fentalogues in the United States, and these compounds are difficult to reliably identify with color-based tests.

In some jurisdictions, safety issues have led to the elimination of presumptive drug testing in the field altogether. Instead of testing these unknown substances in the field, law enforcement officers collect them and send them to the forensic laboratory for confirmatory testing. Although the elimination of presumptive field testing kits may improve the safety and efficiency of law enforcement, this change may lead to one or more of the following effects: (1) more individuals may be arrested on drug charges if unknown substances cannot be tested in the field, which could increase the number of plea deals; (2) prosecutors may see a decrease in plea deals, increasing their caseload and leading to longer wait times until trials; or (3) forensic

Check out "Opioid Crisis- A Public Health Enemy Webinar Series," produced by the FTCoE. "Strategies and Considerations for Trace Detection of Fentalogs" and "Regional Fentanyl Trends, Safety, & Field Testing" both discuss the use of field portable devices in presumptively identifying fentanyl.

laboratories may have higher caseloads as field-based testing is shifted to the laboratory, and more drug-related cases may go to trial and require confirmatory laboratory results for convictions.

When choosing whether to eliminate field testing altogether, law enforcement agencies should consider specific factors within their criminal justice system, including the following:

- **Establishing probable cause**—One role of these presumptive field tests is to establish probable cause to arrest an individual suspected of possessing illicit drugs. If presumptive tests are eliminated, these jurisdictions will have to rely on other factors to justify an arrest, which may require changing or developing regulations surrounding arrest procedures.
- **Prevalence of dangerous drugs**—Agencies in areas that see a large number of fentanyl seizures, such as the eastern United States, may consider eliminating field testing for officer safety [27].

• Turnaround time for laboratory/lab capacity—Agencies with a short turnaround time for confirmatory drug testing may not need presumptive testing because their laboratories can provide results rapidly, expediting the criminal justice process. Conversely, eliminating presumptive testing can lead to significant laboratory caseload increases, which could delay cases, as experienced by the Arizona Department of Public Health [28-30].

Examples of Agencies Eliminating Field Testing

The Arizona Department of Public Safety recently eliminated presumptive drug testing in 2017 in response to concerns about officer safety and fentanyl. After elimination, a backlog of more than 2,000 cases not tested within 30 days built up [28]. This example highlights the delicate balance between safety and efficiency that must be weighed when considering whether to implement or eliminate presumptive field testing.

In contrast, the Houston Forensic Science Center in Texas and Redlands Police Department in California have eliminated field testing as a requirement for accepting charges without significantly affecting lab turnaround time. In Houston, this measure was a coordinated effort by the DA's office, forensic laboratory, and law enforcement agencies. Agencies were provided clear guidelines for arresting an individual without using field tests and have ceased prosecuting cases where a trace amount of an unknown substance is found, which has reduced the caseload for laboratories, enabling quick turnaround time.

The downstream effects of eliminating field testing are highly variable between jurisdictions based on their unique circumstances, such as their average laboratory turnaround time, and the decision requires careful consideration from multiple stakeholders.

Landscape of Portable Technologies for Presumptive Testing in the Field

Many types of products are available to support presumptive drug testing in the field. All these instruments have been adapted from laboratory instruments for field use. This section provides an overview of the technologies, descriptions of how they work, their benefits and limitations, and a snapshot of related products that are available for purchase. Specifically, this section highlights MS, IMS, and spectroscopy (including Raman and IR).

For a comprehensive list of manufacturers and their portable devices for presumptive drug testing in the field, please see the Appendix.

Mass Spectrometry

MS is a technique used to identify compounds based on their molecular construction. Individual molecules are ionized to form either positive or negative ions, which are then accelerated into a mass analyzer [8]. The mass analyzer separates these ions based on their mass-to-charge ratio (m/z) and determines the molecular weights of the molecules. Many mass spectrometers apply additional energy to the molecular ions to break them into smaller fragments before they enter the mass analyzer. Compounds can be identified based on their intact molecular weights and fragmentation patterns or by comparing their spectra

to those of known standards within a reference library. The advantages and disadvantages of MS for presumptive drug testing applications are listed in **Exhibit 6**.

MS is a technique that can be used alone (direct analysis) or in tandem with another instrument, such as a gas chromatograph (GC) or liquid chromatograph (LC) [8]. Portable MS systems operate in different ways, depending on the manufacturer, model, and sample introduction method. Currently available products are described in **Exhibit 10**. Samples of interest can be introduced into a mass spectrometer in the solid, liquid, and/or gas phase based on the capabilities of the particular instrument. Some models may have accessories to adapt to different uses and types of samples. Some of the most common sample introduction methods used in portable mass spectrometers are listed below. Not all methods are compatible with all

Gas Chromatography-Mass Spectrometry (GC-MS)

- ► GC-MS is a commonly used method in the laboratory for drug analysis.
- ► This technique is useful because the substance of interest is separated before ionization based on a number of factors (e.g., the boiling point and polarity of compound, temperature, and the composition and length of the chromatographic column).
- ▶ Libraries, such as the NIST library, are readily available to assist with identifying unknown samples.

instruments, and each type of sample introduction method requires a different amount of sample preparation to achieve results.

- Vapor-phase introduction: real-time detection of chemicals present in the air.
- SPME: allows for a solvent-free way to collect a sample prior to analysis by using a polymer-coated fiber to extract the compounds of interest through absorption [31].
- GC: allows for separation prior to ionization, with solid, liquid, or gas sample introduction possible, depending on the model.

Use of Portable Ambient Mass Spectrometry in Crime Scenes

NIJ grantee Chris Mulligan of the University of Illinois (2011-DN-BX-K552) developed a portable MS detector that uses ambient ionization methods. Mulligan explored the reliability, reproducibility, selectivity, and sensitivity of the instrument compared to current methods. Read more about his research here.

Exhibit 6. Advantages and disadvantages of mass spectrometry

Pros Cons

- Mixture identification
- Solid-phase micro extraction (SPME) and vapor introduction methods facilitate little to no sample preparation
- MS: SWGDRUG/ASTM Category A (MS) [1, 32]
- GC-MS: SWGDRUG/ASTM Category B + A [1, 32]
- Ideal for
 - Mixtures
 - Powders
 - Trace amounts

- Difficult to distinguish between isomers
- Destructive method
- Cannot sample through packaging
- Sample preparation required (model dependent)
- Knowledge and understanding of technology often necessary
- Possible to overload instrument with too much sample
- Not ideal for
 - Vegetative samples (e.g., marijuana or synthetic marijuana) if not fully dissolved in solvent

Ion Mobility Spectrometry

IMS is a technique that uses an electric field to separate gas-phase ions based on their mobility. The compound of interest is first volatilized and ionized under ambient conditions (i.e., no vacuum is required); then, the resulting ions are pulled through a drift tube by an electric field while being pushed against a gas in the tube. The ions are separated as smaller ions travel down the tube quicker than larger ones [33].

As IMS technology has improved, the instruments have become more portable and applicable for field use. Field-portable IMS technology can provide either a spectrum for advanced users or a red light/green light approach for easier use by police officers or other field-based personnel who are not experts. **Exhibit 7** presents the advantages and disadvantages of IMS for field use, and **Exhibit 11** lists currently available products.

Exhibit 7. Advantages and disadvantages of IMS

Pros Cons

- Can sample the outside of a package for trace quantities
- Mixture detection
- Simple use (red light/green light)
- SWGDRUG/ASTM Category B [1, 32]
- Ideal for
 - Mixtures
 - Trace amounts

- Sensitivity can cause delays in processing because of sample overload.
- Not ideal for
 - Tetrahydrocannabinol (THC) because it is thermally labile and difficult to vaporize

Spectroscopy

Spectroscopic techniques measure how a sample absorbs and emits light to gain information about that sample's molecular structure. The two most common types of spectroscopy used in drug identification are Raman and IR spectroscopy.

In most portable Raman and IR devices, a spectrum of an unidentified sample is collected and then compared to an onboard library of reference spectra. In this scenario, the spectroscopic device is limited to identifying compounds for which a reference spectrum is available. Because of this, many manufacturers offer regular updates to onboard libraries or allow users to add their own reference spectra. A trained spectroscopist can interpret IR and Raman spectra directly, without comparison to a reference spectrum. Thus, these technologies can be useful for NPSs, for which reference material often does not exist, given appropriate scientific expertise or reachback support from a manufacturer.

Raman Spectroscopy

Raman spectroscopy is a form of vibrational spectroscopy. In Raman spectroscopy, a sample is irradiated with light (usually a laser) at a specific wavelength. A small amount of that light, typically less than 0.001%, is scattered at a different wavelength, in a manner known as Raman scattering. The Raman-scattered light is collected with a lens and sent through an interference filter or spectrophotometer to obtain the sample's Raman spectrum, which is characteristic for a specific molecular structure. Using Raman, identifying samples that fluoresce under laser light, such as heroin and marijuana, is difficult because the fluorescence signal is typically much stronger than the Raman scattering. Dark samples are also problematic because they can absorb energy from the laser light and heat to the point of burning. Portable Raman systems usually operate using a point-and-shoot method, in which the sample is placed on a flat surface, the Raman device is directed toward the sample, and analysis proceeds without direct contact with the sample. Exhibit 8 presents the advantages and

Additional Raman Resources

For more information on purchasing and implementing Raman spectrometers, consult A Landscape Study of Handheld and Portable Raman Spectrometers.

NIJ grantee Stephana Fedchak of the Las Vegas Metropolitan Police Department (2010-DN-BX-K201) evaluated the use of the ReporteR, a field-portable Raman spectrometer, to presumptively identify cocaine and heroin. Read the final report here.

disadvantages of Raman for field use, and Exhibit 12 lists the Raman products that are currently available.

Exhibit 8. Advantages and disadvantages of Raman

Pros Cons

- Non-destructive
- Not subject to interference from water
- Can sample through clear plastic and glass
- Highly selective—SWGDRUG/ASTM Category A [1, 32]
- Ideal for
 - White powders
 - Single-component samples
 - Bulk amounts

- Quite a few drugs exhibit fluorescence in common Raman wavelengths, which can limit results
- Dark targets or surfaces absorb energy, which can alter the results or damage the sample
- Laser wavelength in instrument may require added safety measures
- Not ideal for
 - Dark samples
 - Vegetative samples (e.g., marijuana or synthetic marijuana)
 - Mixtures with components <5% (trace amounts)

Infrared Spectroscopy

IR is also a form of vibrational spectroscopy. In IR, a sample is irradiated with light consisting of multiple wavelengths in the IR region (750 nm to 1 mm). As the IR radiation passes through the sample, some of it is absorbed, depending on the molecular structure of the sample. The amount of light absorbed at each wavelength is measured, and the results are used to generate an IR spectrum, which is characteristic of a specific molecular structure. Most modern IR spectrometers include an interferometer in the source to improve the signal-to-noise ratio. The interferometer performs a mathematical calculation known as a Fourier transform to convert the detected signal into an easily interpretable spectrum; this technique is known as FTIR.

Portable IR systems operate as either point-and-shoot or table-top devices. When using point-and-shoot IR devices, a sample is placed on a flat surface, the IR device is aimed at the sample, and analysis proceeds without direct contact with the sample. In point-and-shoot devices with an ATR sampling interface, the sample must be in contact with the IR instrument. When using table-top devices, a small amount of sample is removed and placed on a sampling surface that is part of the IR device. **Exhibit 9** presents the advantages and disadvantages of IR for field use, and **Exhibit 13** lists the IR products that are currently available.

Exhibit 9. Advantages and disadvantages of IR

Pros Cons

- Non-destructive
- Highly selective—SWGDRUG Category A [1, 32]
- Ideal for
 - White powders
 - Single-component samples

- Samples must be able to allow light to pass through
- Strong interference from moisture in samples
- Not ideal for
 - Mixtures with components <5%
 - Thick or opaque samples

Exhibit 10. Currently available MS products for presumptive drug testing

			C	Gas Chromatography	- Mass Spectrometi	ту			Mass Spectrometry	
	Brı	ıker		FLIR Sy	ystems		PerkinElmer	Smiths Detection	BaySpec	
Model	MM2	E ² M	Griffin G410	Griffin G460	Griffin G465	Griffin G510	Torion T-9	GUARDION	Portability	
			d d	8 8				EBBO F		
					Cost/Availability					
Price (per Instrument)	\$\$\$\$\$	\$\$\$\$\$	\$\$\$\$ \$	\$\$\$\$ \$	\$\$\$\$ \$	\$\$\$\$ \$	\$\$\$\$\$	\$\$\$\$\$	\$\$\$\$\$	
Leasing Available?	No	No	No	No	No	*	via third party	*	No	
	Physical Specifications									
Weight	77 lbs.	68 lbs.	80.5 lbs.	98 lbs.	99.5 lbs.	36 lbs.	32 lbs.	32 lbs.	22 lbs.	
Dimensions (LxWxH in inches)	17.3 x 12.1 x 17.3	17.3 x 14.2 x 17.7	19.7 x 20.3 x 17.8	19.2 x 19.2 x 21.1	19.2 x 19.2 x 21.1	13.25 x 13.25x 15.75	15 x 15.7 x 9.0	15.4 x 15 x 8.7	13 x 9 x 16.1	
Power Source	plug-in	plug-in	plug-in	plug-in	plug-in	plug-in and battery	battery	plug-in and battery	plug-in and battery	
Battery Life	N/A	N/A	N/A	N/A	N/A	2 – 4 hours	2.5 hours	2 – 3 hours	2 – 3 hours	
Ruggedization	MIL Spec	*	MIL-STD-810G; internal shock mounting system; no external shock table required	MIL-STD-810G; internal shock mounting system; no external shock table required	MIL-STD-810G; internal shock mounting system; no external shock table required	IP65-rated enclosure is dust-tight and spray- resistant	minimal openings for typical outdoor conditions	sealed system for operation in hot zone and extreme conditions	metal case for function during transportation up to 50 mph	
Operating Temp. Range	-32°C – 49°C (-25.6°F – 120.2°F)	5°C – 45°C (41°F – 113°F)	5°C – 40°C (41°F – 104°F)	5°C – 40°C (41°F – 104°F)	5°C – 40°C (41°F – 104°F)	0°C – 40°C (32°F – 104°F)	5°C – 45°C (41°F – 113°F)	0°C – 45°C (32°F – 113°F)	5°C – 40°C (41°F – 104°F)	
Onboard Control/ External Control	requires laptop for operation	requires laptop for operation	partial onboard controls, full automation by computer connection	partial onboard controls, full automation by computer connection	partial onboard controls, full automation by computer connection	9" onboard touchscreen display; can be operated while wearing PPE	color touchscreen; can be operated while wearing PPE.	touchscreen embedded system; finger, stylus, or keypad navigation	touchscreen with Windows 7 embedded system	
Spectra Display on Unit	No	No	No	No	No	Yes	Yes	Yes	Yes	
					Operation					
Sample Format/ Introduction (Standard)	syringe injection, SPME	solid, liquid, vapor	syringe injection (additional methods via optional accessories)	syringe injection, direct air intake (additional methods via optional accessories)	syringe injection, direct air intake (additional methods via optional accessories)	syringe injection, direct air intake (additional methods via optional accessories)	SPME and needle trap	SPME; headspace; Tedlar® bag; liquid; solution (gas, liquid, solid)	thermal desorption probe	
Vacuum System	Yes, details not specified	Yes, details not specified	turbomolecular and diaphragm pumps	turbomolecular roughing pumps	turbomolecular diaphragm pump	integrated in MS system				
Carrier Gas Type/ Containment	N/A	N/A	He or H ₂ : Connection for external gas source	He or H ₂ : Connection for external gas source	He or H ₂ ; Connection for external gas source	He or H ₂ ; internal cartridge and external helium connector; automatic switching	~150 analyses/onboard He cylinder	He carrier gas supply; internal disposable cartridge or external cylinder	internal gas sampling pump using ambient air	
Calibrant	Yes	Yes	onboard PFTBA	onboard PFTBA	onboard PFTBA	onboard PFTBA	13 mix standard	*	No	

			G	as Chromatography	- Mass Spectrometi	у			Mass Spectrometry
	Bru	ıker		FLIR Sy	ystems		PerkinElmer	Smiths Detection	BaySpec
Model	MM2	E ² M	Griffin G410	Griffin G460	Griffin G465	Griffin G510	Torion T-9	GUARDION	Portability
Alarm	audible and visible	audible and visible	visible	visible	visible	audible and visible	visible	Yes	visible
Warm-up Time	30 minutes	30 minutes	30 minutes	30 minutes	30 minutes	15 minutes	>5 minutes	<5 minutes	~5 minutes
Analysis Time	vapor mode <1 min. GC attached ~15 mins.	vapor mode <1 min. GC attached ~15 mins.	4-15 minutes	4-15 minutes	4-15 minutes; real-time in survey mode	4-15 minutes; real-time in survey mode	5 minutes	<3 minutes	~10 seconds
Mixture Detection and Method	Yes	Yes	Yes, capillary GC separation	Yes, capillary GC separation	Yes, capillary GC separation	Yes, capillary GC separation	Yes, deconvolution algorithm	Yes	Yes, MS/MS capable
Radioactive Ionization Source	Yes	Yes	No	No	No	No	No	*	No
Ionization Type	electron impact	electron impact	electron impact	electron impact	electron impact	electron impact	electron impact	electron impact	electrospray; atmospeheric pressure chemical
Mass Range	1 – 520 m/z	1 – 520 m/z	35 – 425 m/z	35 – 425 m/z	35 – 425 m/z	15 – 515 m/z	41 – 500 m/z	50 – 500 m/z	70 – 650 m/z
Mass Analyzer	quadrupole	quadrupole	MS/MS-capable ion trap	MS/MS-capable ion trap	MS/MS-capable ion trap	linear quadrupole toroidal ion tra		toroidal ion trap	miniature linear ion trap (LIT)
Data Output	spectra, PDF report	spectra, PDF report	mass spectra	mass spectra	mass spectra	mass spectra	CHROMION (spectra, chromatograms, etc.)	CHROMION advanced GC/ MS software	spectra or red light/green light approach, based on user
Output Method	operated via laptop so networking and printer are available	operated via laptop so networking and printer are available	external laptop control	external laptop control	external laptop control	onboard computer, WiFi, USB, Bluetooth	ethernet	onboard removable SD flash card; standard, mini- USB ports	can be wirelessly attached to printer
					Resources/Add-ons				
Library Type	toxic chemicals and chemical warfare agents; GC-MS data is NIST searchable	toxic chemical; GC-MS data is NIST searchable	GriffinLib, NIST	GriffinLib, NIST	GriffinLib, NIST	GriffinLib, NIST	onboard library, NIST compatible	NIST/EPA/NIH Mass Spectral Library	*
Library Updates	user customizable	user customizable	user customizable and central library updates	user customizable and central library updates	user customizable and central library updates	user customizable and central library updates	user customizable	user customizable	user customizable
Network Connection	ethernet to control laptop	ethernet to control laptop	ethernet TCP/IP; remote operation and diagnostics	ethernet TCP/IP; remote operation and diagnostics	ethernet TCP/IP; remote operation and diagnostics	Bluetooth 4.0, WiFi 802.11n, ethernet via USB, integrated GPS	ethernet, USB	Bluetooth	WiFi, ethernet, USB
Accessories and/ or Equipment Options	air sampling probe, GC, shock mount, surface sampler, wheel monitoring	air sampling probe, GC, surface sampler	Griffin X-Sorber, SPME fiber, Griffin Purge & Trap, autosampler, PSI-probe, headspace sampler, etc.	Griffin X-Sorber, SPME fiber, Griffin Purge & Trap, autosampler, PSI-probe, headspace sampler, etc.	Griffin X-Sorber, SPME fiber, Griffin Purge & Trap, autosampler, PSI-probe, headspace sampler, etc.	SPME fiber, PSI-probe, headspace sampler	SPME syringe, sample prep station (SPS-3) and needle trap	thermal desorber unit, SPME holders, SPME fibers, computer	2 possible external ionization sources
Warranty	Yes	Yes	extended warranties available up to 5 years	extended warranties available up to 5 years	extended warranties available up to 5 years	extended warranties available up to 5 years	1 year included	extended warranty available up to 3 years	1 year included
Training Available?	Yes	Yes	Yes	Yes	Yes	Yes, included	Yes	Yes, included	Yes

^{*} Manufacturer did not provide requested information (or was not consistent with information from other manufacturers). Please contact manufacturer for information.

Exhibit 11. Currently available IMS products for presumptive drug testing

				on Mobility Spectrometry	/		
	Bru	ıker	L3 Security and Detection		Smiths D	etection	
Model	RAID M-100	Roadrunner	B220	lonScan 500DT	IonScan 600	Sabre 5000	MMTD
					omcanes o		
				Cost/Availability			
Price (per Instrument)	\$\$ \$\$\$	\$\$\$ \$\$	\$\$\$\$ \$	\$\$\$\$ \$	\$\$\$ \$\$	\$\$\$ \$\$	\$\$\$\$ \$
Leasing Available?	No	No	No	via third party	via third party	via third party	via third party
				Physical Specifications			
Weight	7.7 lbs.	7.5 lbs.	32.1 lbs.	43 lbs.	23.8 lbs.	7 lbs.	12.3 lbs.
Dimensions (LxWxH in inches)	17.3 x 15.0 x 6.9	13.9 x 5.0 x 12.4	15.6 x 14.4 x 16.2	16.0 x 12.5 x 16.0 (closed) 16.0 x 22.5 x 16.0 (open)	14.8 x 12.0 x 12.9	14.5 x 4.0 x 4.5	19.0 x 8.5 x 8.0
Power Source	plug-in and battery	plug-in and battery	plug-in	plug-in	plug-in and battery	plug-in and battery	plug-in and battery
Battery Life	*	3.2 hrs	N/A	N/A	1 hour (hot swappable)	4 hours	5 hours
Ruggedization	MIL-STD-810F	No	No	portable	portable	portable	IP54/IP53
Operating Temp. Range	-30°C – 50°C (-22°F – 122°F)	0°C – 40°C (32°F – 104°F)	-10°C – 55°C (14°F – 131°F)	0°C - 40°C (32°F - 104°F)	-10°C – 50°C (14°F – 122°F)	0°C - 40°C (32°F - 104°F)	-7°C – 55°C (20°F – 131°F)
Display	background illuminated display	4.5" on diagonal	12.5" high-resolution color touchscreen	10.4" color touchscreen	9" high resolution, anti-reflective, color touchscreen	3.5" color TFT LCD	3.5" color TFT LCD
Spectra Display on Unit	Yes	Yes	Yes	Yes	No	Yes	Yes
				Processing			
Sample Format/ Introduction	point detectors	wipe and vapor point detection	wipe	swab	swab	swab, direct air	swab, direct air
Sensitivity	*	*	nanogram	~1 ng	~1 ng	low-ng range	low-ng range
Calibrant	internal calibration	internal calibration	inCal automatic internal calibration system	nicotinamide	nicotinamide and others	nicotinamide	nicotinamide
Alarm	audible and visible	audible and visible	audible and visible	audible and visible	audible and visible	audible and visible	audible and visible
Warm-up Time	15 minutes	30 minutes	30 minutes	30 minutes	<10 minutes	<15 minutes	<10 minutes
Analysis Time	*	20 seconds	>10 seconds	5-8 seconds	<8 seconds	<20 seconds	<10 seconds
Mixture Detection	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Radioactive Ionization Source	Yes	No	No	Yes	No	Yes	Yes

				on Mobility Spectrometry	/						
	Bru	ker	L3 Security and Detection		Smiths Detection						
Model	RAID M-100	Roadrunner	B220	IonScan 500DT	IonScan 600	Sabre 5000	MMTD				
Ionization Type	Nickel - 63	high energy photoionization	photonic	APCI	APCI	APCI	APCI				
Data Output	spectra, text files	spectra, text files	spectra	identification, plasmagram	identification, summary of peak intensities	identification, plasmagram	identification, plasmagram				
Output Options	connection to a laptop	connection to a laptop	printer, network	built-in printer	built-in printer	export to PC	export to PC				
Resources/Add-ons											
Library Type	toxic chemicals and chemical warfare agents	narcotics and explosives	narcotics and explosives	drugs of abuse including featanul		drugs of abuse	drugs of abuse				
Library Updates	user customizable	user customizable	user customizable	user customizable and central library updates	user customizable and central library updates	user customizable and central library updates	user customizable and central library updates				
Network Connection	No	ethernet, USB	ethernet, USB	ethernet	ethernet	USB	USB, SD card				
Accessories and/ or Equipment Options	various	various	wand, gloves	*		*	*				
Safety Considerations	radioactive source	No	No	subject to nuclear regulatory shipping and maintenance requirements	No	subject to nuclear regulatory shipping and maintenance requirements	subject to nuclear regulatory shipping and maintenance requirements				
Warranty	Yes	Yes	1 year included	available	available	available	available				
Training Available?	Yes	Yes	Yes	Yes	Yes	Yes	Yes				

^{*} Manufacturer did not provide requested information (or was not consistent with information from other manufacturers). Please contact manufacturer for information.

Exhibit 12. Currently available Raman products for presumptive drug testing

					Raman Sp	ectroscopy				
	B&V	V Tek	Coda Devices	Field Forensics	Real-Time Analyzers	SciAps		ThermoFish	er Scientific	
Model	TacticID-GP	TacticID-N	CDI 1M (mobile)	HandyRam	RamanID	Inspector 500	TruNarc	FirstDefender RM	FirstDefender RMX	Gemini
	100 Control of the co			Headness more leaves to the second leaves to the se		Scripp	Carloctanii	The state of the s		
					Cost/Av	ailability				
Price (per Instrument)	\$\$\$\$ \$	\$\$ \$\$\$	\$ \$\$\$\$	\$\$ \$\$\$ - \$\$\$ \$\$	\$\$\$\$\$	\$\$\$\$ \$	\$ \$\$\$\$ - \$\$ \$\$\$	\$\$\$\$ \$	\$\$\$\$\$	\$\$\$\$\$
Leasing Available?	No	No	Yes, \$599/mo	Yes, starting at \$2000/ mo	No	*	*	*	*	*
					Physical Sp	ecifications				
Weight	2 lbs.	2 lbs.	11.7 lbs.	1.2 lbs.	30 lbs.	3.7 lbs.	1.25 lbs.	< 1.8 lbs.	< 2.0 lbs.	4.2 lbs.
Dimensions (LxWxH in inches)	7.5 x 3.9 x 2.0	7.5 x 3.9 x 2.0	18 x 11.4 x 4.2	3.8 x 3.2 x 1.8	20 x 16 x 8	7.5 x 6.9 x 1.7	6.4 x 4.1 x 2.0	7.6 x 4.2 x 1.75	7.7 x 4.2 x 2.4	10.1 x 5.7 x 2.4
Power Source	plug-in and battery	plug-in and battery	plug-in and battery	battery	plug-in and battery	battery	battery	battery	battery	plug-in and battery
Battery Life	>10 hours	>10 hours	10 hours	~4 hours	5 hours	4 hours	> 10 hours	> 4 hours	> 4 hours	*
Ruggedization	MIL-STD-810G IP65	MIL-STD-810G IP65	millitary-grade case, IP67	MIL-STD-810G IP67	sealed surface; CBN decontamination when closed	MIL-STD-810G IP67	IP64	MIL-STD-810G IP67	MIL-STD-810G IP67	MIL-STD-810G IP67
Operating Temp. Range	-20°C – 50°C (-4°F – 122°F)	-20°C – 50°C (-4°F – 122°F)	-10°C – 40°C (14°F – 104°F)	-20°C – 40°C (-4°F – 104°F)	0°C – 43°C (32°F – 110°F)	-20°C – 40°C (-4°F – 104°F)	-10°C – 50°C (14°F – 122°F)	-20°C – 50°C (-4°F – 122°F)	-20°C – 50°C (-4°F – 122°F)	*
Display	color LED touchscreen	color LED touchscreen	color LED touchscreen	LCD with Resistive Touchscreen (2.8")	color LED Screen	color LED touchscreen	color LED	color LED	color LED	*
Spectra Display on Unit	Yes	Yes	Yes	Yes	Yes	*	No	Yes	Yes	*
					Oper	ation				
Sample Format/ Introduction	point and shoot	point and shoot	baggies, vials should be placed on an analytical window	point and shoot; vial adapter	fixed sample holder for 2 or 20 mL glass vials	point and shoot; fixed sample holder	point and shoot	point and shoot; integrated vial	point and shoot; integrated vial	*
Sensitivity	varies depending on sample, sometimes less than a milligram	varies depending on sample, sometimes less than a milligram	amount needed to cover area of 1.5mm^2	~10mg	*	*	*	*	*	*
Alarm	audible and visible	audible and visible	audible and visible (optional)	No	No	*	*	*	*	*
Warm-up Time	~0.5 minutes	~0.5 minutes	0.2 minutes	0.5 minutes	1 minute	*	*	*	*	2 minutes
Analysis Time	> 1 second	> 1 second	10 – 30 seconds	30 seconds	10 – 60 seconds	*	*	*	*	< 40 seconds

					Raman Spe	ectroscopy				
	B&V	V Tek	Coda Devices	Field Forensics	s Real-Time SciAps ThermoFisher Scientific			ner Scientific		
Model	TacticID-GP	TacticID-N	CDI 1M (mobile)	HandyRam	RamanID	Inspector 500	TruNarc	First Defender RM	FirstDefender RMX	Gemini
Mixture Detection and Method	Yes, capable of identifying key components	Yes, capable of identifying key components	Yes, identifies up to 4 components and delivers mixture makeup and relative strengths	Yes, proprietary algorithm	N/A	Yes, proprietary algorithm	Yes, identifies up to 2 component alarm items or clear item mixtures	Yes, automatic mixture analysis & identification of up to 4 components	Yes, automatic mixture analysis & identification of up to 4 components	*
Radioactive Ionization Source	No	No	No	No	*	*	*	*	*	*
Data Output	Spectra, report with ID match, raw data	Spectra, report with ID match, raw data	substance title, amount, class	.SPC, .TXT, .CSV	Spectra	*	*	*	*	*
Output Options	printable PDF report, save to server	printable PDF report, save to server	printed report, network, PDF, CSV, etc.	USB to PC	ethernet/USB	*	*	*	*	*
Spectral Range (cm ⁻¹)	176-2900	176-2900	500-1800		150-3350	150-2450	*	250-2875	250-2875	250-2875
Resolution	9 cm ⁻¹ at 912 nm	9 cm ⁻¹ at 912 nm	6-8 cm ⁻¹	10-12 cm ⁻¹	8, 16, 32 cm ⁻¹	8-10 cm ⁻¹	*	7-10.5 cm ⁻¹	7-10.5 cm ⁻¹	7-10.5 cm ⁻¹
Excitation Laser	785 nm (300 (+-30) mW)	785 nm (300 (+-30) mW)	785 nm		1064 nm (500 mW)	1030 nm (300 mW)	785 nm (250 mW)	75, 125, 250 mW	75, 125, 250 mW	785 nm
					Resources	s/Add-ons				
Library Type	>10,000 Items: Explosives, toxic industrial chemicals, narcotics, cutting agents, precursors, pharmaceuticals	>1,000 Items: Narcotics, cutting agents, precursors, pharmaceuticals	3600 pharmaceuticals, 200+illicits: Pharmaceuticals, illicits, precursors, cutting agents, synthetics, and bath salts	Custom and Commercially Available	ChemID software loaded with 500 spectra in initial library	narcotics, explosives, pharmaceuticals, plastics, minerals	315 items: narcotics, cutting agents, precursors, synthetic cannabinoids and cathinones	12,100 items: explosives, toxic industrial chemicals, chemical warfare agents, narcotics, precursors	12,100 items: explosives, toxic industrial chemicals, chemical warfare agents, narcotics, precursors	13,000 items
Library Updates	user customizable and central library updates	central library updates	user customizable and central library updates	user customizable and central library updates	user customizable	*	central library updates	user customizable and central library updates	user customizable and central library updates	user customizable
Network Connection	WiFi, ethernet, USB	WiFi, ethernet, USB	WiFi, ethernet	USB	USB	Bluetooth	No	No	No	*
Accessories and/ or Equipment Options	point and shoot, vial holder, right angle adapter, SERS adapter	point and shoot, vial holder, right angle adapter, SERS adapter	spatula, sample bags and vials, cleaning supplies, USB LED light, wall and car charger	point and shoot adapter; vial holder; vials for sampling	sample containers	*	*	*	*	*
Warranty	2 years	2 years	1 year	available	1 year	*	*	*	*	1 year
Safety Considerations	laser	laser	Class I system	laser (Class IIIR)	laser	laser	laser	laser	laser	laser
Training Available?	Yes	Yes	Yes, included	Yes	Yes	*	*	*	*	*

^{*} Manufacturer did not provide requested information (or was not consistent with information from other manufacturers). Please contact manufacturer for information.

Exhibit 13. Currently available IR products for presumptive drug testing

		Infrared Spectroscopy							
	Agilent		JASCO		Smiths Detection		ThermoFisher Scientific		
Model	4300 Handheld FTIR	4500 Portable FTIR	VIR-100	VIR-200	Target-ID	HazMatID Elite	TruDefender FT	TruDefender FTi	Gemini
					Cost/Availability				
Price (per Instrument)	\$\$\$\$ \$	\$\$\$ \$\$	\$\$\$ \$\$	\$\$\$ \$\$- \$\$\$\$ \$	*	\$\$\$\$\$-\$\$\$\$\$	\$\$\$\$ \$	*	\$\$\$\$\$
Leasing Available?	via third party	via third party	Yes	Yes	via third party	via third party	*	*	
	Physical Specifications								
Weight	4.15 lbs.	15.0 lbs.	26.5 lbs.	26.5 lbs.	5.4 lbs.	5.05 lbs.	2.9 lbs.	3.4 lbs.	4.2 lbs.
Dimensions (LxWxH in inches)	4.0 x 7.5 x 13.6	8.5 x 11.5 x 7.5	10.7 x 9.4 x 9.7	10.7 x 9.4 x 9.7	10.1 x 6.15 x 3.87	10.6 x 5.6 x 3.1	7.7 x 4.4 x 2.1	7.7 x 4.4 x 2.4	10.1 x 5.7 x 2.4
Power Source	plug-in and battery	plug-in and battery	plug-in and battery	plug-in and battery	plug-in and battery	plug-in and battery	plug-in and battery	plug-in and battery	plug-in and battery
Battery Life	3.5 hours	3.5 hours	*	*	4 hours	4 hours	>4 hours	>4 hours	*
Ruggedization	IP54 and scan capabily in multiple orientations	IP54 standards	Self locking moving mirror, aluminum interferometer housing, steel case, anti vibration technology	Self locking moving mirror, aluminum interferometer housing, steel case, anti vibration technology	No	MIL-STD-810G	MIL-STD-810F IP67 certification	MIL-STD-810G IP67 certification	MIL-810-G IP67 certification
Operating Temp. Range	0°C – 48.9°C (32°F – 120°F)	-10°C - 50°C (14°F - 122°F)	*	*	-10°C - 46.1°C (14°F - 115°F)	-20°C – 50°C (-4°F – 122°F)	-25°C – 40°C (-13°F – 104°F)	-20°C – 40°C (-4°F – 104°F)	*
Onboard Control/ External Control	55x75 mm LCD touchscreen onboard; PC interface optional	8" ruggedized (IP65) tablet included; laptop, desktop optional	No, PC control only (laptop or desktop)	No, PC control only (laptop or desktop)	4.3" LCD color	4.3" LCD color	Yes	Yes	*
Spectra Display on Unit	Yes	No	No	No	*	Yes	*	*	*
Operation									
Sample Format/ Introduction	direct with multiple sampling option	direct, single configuration	direct application by fiber probe, diffuse reflectance, specular reflectance, transmittance or ATR	direct application by fiber probe, diffuse reflectance, specular reflectance, transmittance or ATR	*	integrated solids press and liquids well; direct via ATR	*	*	*
Sensitivity	mg of sample needed, sensitivity sub percent	mg of sample needed, sensitivity sub percent	sample and matrix dependent, parts per hundred to parts per thousand	sample and matrix dependent, parts per hundred to parts per thousand	*	a few milligrams (solids/ pastes/gels); 1 drop (liquid)	*	*	*
Alarm	visible	visible	No	No	*	audible and visible	visible	*	*
Warm-up Time	10 minutes	10 minutes	15–30 minutes	15–30 minutes	<1 minute	<1 minute	<1 minute	<1 minute	2 minutes

		Infrared Spectroscopy							
	Agilent		JASCO		Smiths Detection		ThermoFisher Scientific		
Model	4300 Handheld FTIR	4500 Portable FTIR	VIR-100	VIR-200	Target-ID	HazMatID Elite	TruDefender FT	TruDefender FTi	Gemini
Analysis Time	<2 minutes	<2 minutes	1 second – 10 minutes, (15–30 seconds typical)	1 second – 10 minutes, (15–30 seconds typical)	<1 minute	<1 minute	1 minute	1 minute	< 40 seconds
Mixture Detection and Method	Yes, stored method analysis	Yes, stored method analysis	Yes, software spectral deconvolution and chemometrics	Yes, software spectral deconvolution and chemometrics	*	Yes, proprietary algorithm	Yes, details not provided	Yes, details not provided	*
Data Output	spectra in standard format, generated reports	spectra in standard format, generated reports	spectra, time course	spectra, time course	*	spectra	spc, txt, jpg	spc, txt, jpg	spc, reachback (rbk), txt, pdf
Output Options	printed, local storage	printed, local storage	data file or printed	data file or printed	*	PC export	*	SMS text, email	*
Spectral Range (cm ⁻¹)	4500-650 (DGTS) 5000-1050 (MCT)	4000-650	7800-350	7800-350	4000-650	4000-650	4000-650	4000-650	4000-650
Resolution	2 cm ⁻¹	4-32 cm ⁻¹	0.9-16 cm ⁻¹	0.4-16 cm ⁻¹	4 cm ⁻¹	4 cm ⁻¹	4 cm ⁻¹	4 cm ⁻¹	4
					Resources/Add-ons				
Library Type	Forensic including drugs, explosives, food additives. All STJapan ATR libraries.	Forensic including drugs, explosives, food additives. All STJapan ATR libraries.	Sadtler KnowItAll, up to 250,000 spectra in segmented libraries	Sadtler KnowItAll, up to 250,000 spectra in segmented libraries	up to 2,500 substances, including synthetic designer drugs	~10,000 spectra including emerging designer drugs, fentanyl and derivatives	12,000 items	*	13,000 items
Library Updates	user customizable	user customizable	user customizable and central library updates	user customizable and central library updates	user customizable	user customizable and central library updates	user customizable	*	user customizable
Network Connection	No	No	USB	USB	*	USB, RF wireless	*	cellular	*
Accessories and/ or Equipment Options	different sample heads; interchangable ATR, specular and diffuse reflection	different sample heads; dedicated unit - ATR, liquid dialpath	IQ Accessory™, Fiber interface, long path gas cell, single reflectance ATR, NIR Specular reflectance, IRT-1000 micro IR, autosampler, transmission measurement, MultiChambIR	IQ Accessory™, Fiber interface, long path gas cell, single reflectance ATR, NIR Specular reflectance, IRT-1000 micro IR, autosampler, transmission measurement, MultiChambIR		advanced software package for data management and upgrade library entries to up to 35,000 spectra; clear sampler	•	*	*
Warranty	1 year included	1 year included	1 year	1 year	*	Yes	1-5 year	*	1 year
Safety Considerations	No	No	Class 1 safety HeNe laser and ceramic source	Class 1 safety HeNe laser and ceramic source	*	No	*	*	laser
Training Available?	Yes	Yes	Yes, included	Yes, included	*	Yes	*	*	*

^{*} Manufacturer did not provide requested information (or was not consistent with information from other manufacturers). Please contact manufacturer for information.

Emerging Presumptive Field Testing Technologies

Beyond the technologies profiled in this report, many other promising technologies exist that could be adapted for field testing of drugs of abuse. These range from emerging technologies that are in the process of being developed from research laboratories into commercial systems to fully developed portable devices that have not been applied to the detection of drugs. Interviews with experts about portable presumptive drug testing offered predictions for the future of presumptive drug testing, as described below.

Technology combinations—Devices that combine two different analytical approaches may be developed to reap the benefits of each approach and overcome their individual shortcomings. Current portable combinations of different technologies include GC-MS and FTIR-Raman (the Gemini, offered by ThermoFisher), and future devices may include combinations such as Raman and IMS, thin layer chromatography (TLC) and IR, and Raman and MS.

Combining technologies can **enable mixture separation**- Because of the proliferation of complex mixtures and multiple isomers of NPSs, devices that include separatory capabilities that are better suited for mixture identification are needed. Next-generation devices may couple GC with spectroscopic methods, such as Raman and IR. Today, GC-IR instruments are commercially available as laboratory -based systems, but no portable versions of this setup have reached the field. Adding more complex analysis to portable TLC devices would also accomplish this goal.

- Safer sampling—Technologies that allow sampling through containers are especially in demand to increase officer safety. Currently, Raman spectrometers are the only commercially available, portable field testing devices that can scan through clear containers. However, promising technologies in this area include near-IR spectroscopy and spatially offset Raman. Near-IR spectroscopy is currently used in the pharmaceutical and food safety fields, and ruggedized portable near-IR instruments are commercially available. For these instruments to be adapted to field drug testing, spectral libraries containing analytical data for drugs that are likely to be encountered must be developed. Near-IR spectra are not as highly resolved as mid-IR spectra for drugs that are likely to be encountered, but the ability to sample through containers and increase officer safety may provide enough incentive to compensate for the decreased signal quality. Spatially-offset Raman spectroscopy can also sample through containers. A ruggedized, handheld, spatially-offset Raman spectrometer is available from Agilent Technologies [34]. This instrument is currently marketed as a narcotics detector, but as of the time of writing this report, we were unable to find instances of any agency using the device for drug testing.
- Advanced detection applications—Researchers are working to deploy laboratory-grade instrumentation in field settings

Check out Episode Eleven: Just One Pot Methamphetamine Synthesis, part of the FTCoE's Just Science podcast series. In this episode, Dr. Jarrad Wagner from Oklahoma State University explains his research in methamphetamine and wastewater effluents.

to improve law enforcement agencies' ability to identify unknown substances. For example, a group at the University of North Texas outfitted a vehicle with a mass spectrometer to prototype a "drug sniffing car," which can detect chemical signatures up to a quarter mile away. This vehicle could facilitate detecting the locations of drug sources such clandestine laboratories within 4% error [35]. In addition, researchers at Oklahoma State are working to detect meth labs through monitoring wastewater effluents.

• Smartphone technologies—Smartphones have the potential to serve as field-portable presumptive drug testing devices. Researchers at UCF developed a handheld spectrometer attachment for smartphones that captures fluorescence of substances under a UV camera and presumptively identifies it based on a cloud-based reference system [36].

Conclusion

The need to quickly and reliably identify unknown substances in field settings has led to the miniaturization and ruggedization of laboratory analysis methods for presumptive drug testing in the field. Agencies looking to adopt these technologies, which offer value beyond traditional color-based testing, currently must choose among four technology types—MS, Raman, IR, and IMS—available in more than 40 commercial devices.

The goal of this landscape study is to enable law enforcement agencies, narcotics units, and other decision makers to make better-informed decisions when purchasing portable presumptive drug testing devices. The information contained herein is derived from current literature and interviews with technology experts, developers, and users in a wide variety of applications. This document provides the reader with background information on the roles and applications of presumptive drug testing in the field, the benefits and limitations of portable presumptive drug testing technologies, considerations for choosing specific types of instruments based on agency- and application-specific factors, specific product details, cases illustrating successful adoption, and predictions for future field testing techniques.

Although law enforcement has employed presumptive drug testing in the field for multiple decades, today's products offer significant advantages over traditional color-based testing, including comprehensive one step testing, objectivity, specificity, safety, chain of custody corroboration, technical support, and versatility.

The FTCoE provides the information in this report to help purchasers and users better select and adopt advanced portable technologies to the benefit of those they serve.

Appendix

The table below presents a list of manufacturers and the portable devices they offer for presumptive field testing applications. Note that all devices are portable but not all are handheld.

Manufacturer	Device Type	Handheld	Devices Profiled
Agilont	IR	Х	4300 Handheld FTIR
Agilent	IR		4500 Series Portable FTIR
BaySpec	MS		Portability
	GC-MS		E2M
Bruker	GC-MS		MM2
bruker	IMS	Χ	RAID M-100
	IMS	Χ	Roadrunner
B&W Tek	Raman	Х	Tactic-ID-GP
DQVV TEK	Raman	Х	Tactic-ID-N
Coda Devices	Raman	Χ	CDI 1M
Field Forensics	Raman	Χ	HandyRam 785R
	GC-MS		Griffin G410
ELID	GC-MS		Griffin G460
FLIR	GC-MS		Griffin G465
	GC-MS		Griffin G510
14500	IR		VIR-100
JASCO	IR		VIR-200
L3	IMS		B220
Perkin Elmer	GC-MS		Torion T-9
RTA	Raman	Х	RamanID
CaiAna	Raman	Х	Inspector 300
SciAps	Raman	Х	Inspector 500
	GC-MS		Guardion
	IMS		IonScan 500DT
	IMS		IonScan 600
Smiths Detection	IMS	Χ	MMTD
Detection	IMS	Χ	Sabre 5000
	IR	Х	Target-ID
	IR	Х	HazMat ID Elite
	IR	Х	FirstDefender RM
	IR	Х	FirstDefender RMX
ThermoFisher	Raman/IR	Х	Gemini
Scientific	Raman	Х	TruDefender FT
	Raman	Х	TruDefender FTi
	Raman	Х	TruNarc

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Information provided herein is intended to be objective and is based on data collected during primary and secondary research efforts available at the time this report was written. Any perceived value judgments may be based on the merits of device features and developer services as they apply to and benefit the law enforcement and forensic communities. The information provided herein is intended to provide a snapshot of current presumptive drug testing device developers and a high-level summary of available devices; it is not intended as an exhaustive product summary. Features or capabilities of additional instruments or developers identified outside of this landscape may be compared with these instrument features and service offerings to aid in the information-gathering or decision-making processes. Experts, stakeholders, and practitioners offered insight related to the use of alternate light sources for law enforcement agencies.