

A Comparative Study of [Device 1] and [Device 2] for the Detection and Identification of Common Drugs of Abuse and Explosives

Forensic Chemistry Research Senior Forensic Chemist University of South Florida (Intern) Massachusetts Institute of Technology (Intern)

Forensic Chemistry Section 8/10/23

Global Forensic and Justice Center (GFJC) Florida International University 8285 Bryan Dairy Rd., Suite 125 Largo FL 33777

### **Executive Summary**

This test report describes the results from a comparison study conducted on behalf of [client] at the Global Forensic and Justice Center (GFJC) located in Largo, FL, from 24 June to 4 August 2023. The Forensic Chemistry section of GFJC at Florida International University (FIU) was tasked to assess [Device 1] compared to [Device 2]. To keep this instrument comparison assessment manageable and completed within a reasonable time, only common illicit drugs, cutting agents and some explosives were used to determine each instruments' specificity, sensitivity, reproducibility, as well as their ability to accurately detect and identify controlled substances in real-world, adjudicated drug case samples. The illicit drugs chosen for this study were based on the most current common drugs of abuse reported by the National Forensic Laboratory Information System (NFLIS) for forensic drug chemistry and toxicology.

To evaluate specificity, twenty-five (25) single component drug and explosive samples were analyzed using both instruments. The objective was to determine the instruments' ability to accurately identify and differentiate between different common drug and explosive compounds, ensuring minimal false positive or false negative detection and identification. To assess inter and intraday reproducibility, a four (4) component polydrug mixture was analyzed for three (3) replicates over a five (5) day period on each instrument. This portion of the comparison study examined the consistency of results generated by each instrument, which proved insight into their reliability and precision.

Sensitivity was evaluated using ten (10) controlled substances and five (5) explosives. The fifteen (15) total single component samples were prepared at varying concentrations from certified standards, allowing the assessment of the instruments' ability to detect and identify low levels of these substances. This area of the assessment provided an understanding of each instrument's limits of detection (LOD) and overall sensitivity for the analytes of interest. Fifteen (15) drug case samples were analyzed using both instruments to evaluate their practical applicability in real-world scenarios. The drug samples used represent diverse matrices commonly encountered in forensic investigations. This final area of the study focused on each instruments ability to accurately detect and identify the drugs of interest in complex matrices, simulating the challenges faced during operation of these devices while in the field.

In order to evaluate and make direct comparisons among the data acquired from each chemical detection device utilized in the four (4) assessment areas as described above, the results were first tabulated and then assigned color designators based on a predefined set of criteria. The assigned color was determined by the device's capacity to successfully detect, identify, and alarm on a singular chemical.

In all scenarios, if the instrument was presented with a sample containing only a single component, a green color was granted if the instrument accurately detected and identified the intended target. In instances where the instrument encountered samples containing multiple compounds, each individual compound within the mixture was given equal weight.

Additionally, a color of yellow was allocated for any correctly SUSPECT chemical identified by [Device 2]. Similarly, this color was also awarded for any chemical identified by [Device 1] that necessitated manual integration for detection, along with user library searching for proper identification. A red color was issued if a chemical component in the sample was misidentified, an orange color for multiple possible alarms ([Device 2] only), and gray if the target chemical was not detected.

Scoring	Device 1	Device 2
	Chemical detected and identified	Chemical detected with confidence
	Chemical detected but not flagged, user search required	Chemical detected with suspect
	N/A	Multiple possible alarms
	Chemical detected but misidentified, or co-detection of an unexpected chemical component	Chemical detected but misidentified
	Not detected, or signal below acceptable thresholds	No target detected or no signal
	No results	No results

A single [Device 1] (Serial No. ---- - ----) and [Device 2] (Serial No. ---- - ---) was used across all four (4) areas of this comparison study. All sample preparation and analysis were performed according to each instruments' manufacturer guidelines using their respective consumables. Both instrument manufacturers have procedures for handling samples where a target chemical is not detected, which requires running a more concentrated sample. This approach was only performed during the sensitivity portion of the assessment and not at any other time.

Several compounds selected for this comparative analysis and subsequently subjected to testing were indicated as "NO TARGET DETECTED" by the [Device 2], despite the presence of observable signals. This discrepancy can be attributed to the limited onboard library of [Device 2]. To ensure the reader has a comprehensive and complete comparison assessment between the instruments, two alternative result summary tables were compiled.

In Table 2, an inclusive overview of the achieved outcomes for all chosen and evaluated compounds is provided. Conversely, Table 3 presents a summary of results solely for compounds that are listed in both devices' libraries. This approach allows for a more focused and equitable assessment between the 2 instruments.

	Device 1				Device 2				
Assessment Area	CORRFCT IDENTIFICATION Automatic	CORRECT IDENIFICATION Manual	MISIDENTIFICATION	NOT DETECTED	CORRECT ALARM ID	CORRECT SUSPECT ID	MULTIPLE POSSIBLE ALARMS	MISIDENTIFICATION	NOT DETECTED
Specificity (25 Compounds)	<b>78.7%</b> (59/75)	<b>5.3%</b> (4/75)	<b>6.7%</b> (5/75)	<b>9.3%</b> (7/75)	<b>56.0%</b> (42/75)	<b>0.0%</b> (0/75)	<b>8.0%</b> (6/75)	<b>0.0%</b> (0/75)	<b>36.0%</b> (27/75)
Intra-Day 1	<b>55.6%</b>	<b>33.3%</b>	<b>0.0%</b>	<b>11.1%</b>	<b>11.1%</b>	<b>22.2%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>66.7%</b>
Reproducibility	(5/9)	(3/9)	(0/9)	(1/9)	(1/9)	(2/9)	(0/9)	(0/9)	(6/9)
Intra-Day 2	<b>44.4%</b>	<b>55.6%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>11.1%</b>	<b>11.1%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>77.8%</b>
Reproducibility	(4/9)	(5/9)	(0/9)	(0/9)	(1/9)	(1/9)	(0/9)	(0/9)	(7/9)
Intra-Day 3	<b>66.7%</b>	<b>11.1%</b>	<b>0.0%</b>	<b>22.2%</b>	<b>22.2%</b>	<b>11.1%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>66.7%</b>
Reproducibility	(6/9)	(1/9)	(0/9)	(2/9)	(2/9)	(1/9)	(0/9)	(0/9)	(6/9)
Intra-Day 4	<b>33.3%</b>	<b>66.7%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>33.3%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>66.7%</b>
Reproducibility	(3/9)	(6/9)	(0/9)	(0/9)	(3/9)	(0/9)	(0/9)	(0/9)	(6/9)
Intra-Day 5	<b>33.3%</b>	<b>55.6%</b>	<b>0.0%</b>	<b>11.1%</b>	<b>22.2%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>77.8%</b>
Reproducibility	(3/9)	(5/9)	(0/9)	(1/9)	(2/9)	(0/9)	(0/9)	(0/9)	(7/9)
Inter-Day	<b>46.7%</b>	<b>44.4%</b>	<b>0.0%</b>	<b>8.9%</b>	<b>20.0%</b>	<b>8.9%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>71.1%</b>
Reproducibility	(21/45)	(20/45)	(0/45)	(4/45)	(9/45)	(4/45)	(0/45)	(0/45)	(32/45)
Real-World Drug Samples (15 Samples)	<b>56.5%</b> (26/46)	<b>13.0%</b> (6/46)	<b>0.0%</b> (0/46)	<b>30.4%</b> (14/46)	<b>32.6%</b> (15/46)	<b>2.2%</b> (1/46)	<b>0.0%</b> (0/46)	<b>2.2%</b> (1/46)	<b>63.0%</b> (29/46)
Sensitivity (Limit of Detection)		ugs 05µg	-	osives )25µg		rugs )62µg	Explosive	s ≥0.031µg	

 Table 2: Summary of Replicate Results For All Selected Compounds Tested On [Device 1] and [Device 2]

I

 Table 3: Summary of Replicate Results for Compounds Listed In Both Devices Libraries

	Device 1				Device 2				
ASSESSMENT AREA	CORRECT IDENTIFICATION Automatic	CORRECT IDENIFICATION Manual	MISIDENTIFICATION	NOT DETECTED	CORRECT ALARM ID	CORRECT SUSPECT ID	MULTIPLE POSSIBLE ALARMS	MISIDENTIFICATION	NOT DETECTED
<b>Specificity</b> (17 Compounds)	<b>80.4%</b> (41/51)	<b>0.0%</b> (0/51)	<b>7.8%</b> (4/51)	<b>11.8%</b> (6/51)	<b>82.4%</b> (42/51)	<b>0.0%</b> (0/51)	<b>11.8%</b> (6/51)	<b>0.0%</b> (0/51)	<b>5.9%</b> (3/51)
Intra-Day 1	<b>33.3%</b>	<b>50.0%</b>	<b>0.0%</b>	<b>16.7%</b>	<b>16.7%</b>	<b>33.3%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>50.0%</b>
Reproducibility	(2/6)	(3/6)	(0/6)	(1/6)	(1/6)	(2/6)	(0/6)	(0/6)	(3/6)
Intra-Day 2	<b>50.0%</b>	<b>50.0%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>16.7%</b>	<b>16.7%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>66.6%</b>
Reproducibility	(3/6)	(3/6)	(0/6)	(0/6)	(1/6)	(1/6)	(0/6)	(0/6)	(4/6)
Intra-Day 3	<b>50.0%</b>	<b>16.7%</b>	<b>0.0%</b>	<b>33.3%</b>	<b>33.3%</b>	<b>16.7%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>50.0%</b>
Reproducibility	(3/6)	(1/6)	(0/6)	(2/6)	(2/6)	(1/6)	(0/6)	(0/6)	(3/6)
Intra-Day 4	<b>33.3%</b>	<b>66.7%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>50.0%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>50.0%</b>
Reproducibility	(2/6)	(4/6)	(0/6)	(0/6)	(3/6)	(0/6)	(0/6)	(0/6)	(3/6)
Intra-Day 5	<b>50.0%</b>	<b>33.3%</b>	<b>0.0%</b>	<b>16.7%</b>	<b>33.3%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>66.6%</b>
Reproducibility	(3/6)	(2/6)	(0/6)	(1/6)	(2/6)	(0/6)	(0/6)	(0/6)	(4/6)
Inter-Day	<b>43.3%</b>	<b>43.3%</b>	<b>0.0%</b>	<b>13.3%</b>	<b>30.0%</b>	<b>13.3%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>56.7%</b>
Reproducibility	(13/30)	(13/30)	(0/30)	(4/30)	(9/30)	(4/30)	(0/30)	(0/30)	(17/30)
Real-World Drug Samples (11 Samples)	<b>63.9%</b> (23/36)	<b>13.9%</b> (5/36)	<b>0.0%</b> (0/36)	<b>22.2%</b> (8/36)	<b>41.7%</b> (15/36)	<b>2.8%</b> (1/36)	<b>0.0%</b> (0/36)	<b>2.8%</b> (1/36)	<b>58.3%</b> (21/36)

# Instrumentation Specifications and Technology Description

Table 4: Instrumentation	Specification	Comparison
--------------------------	---------------	------------

Specification	Device 1	Device 2						
Chemical Separation Technology	Gas Chromatography (High compound separation capability)	Thermal Desorption (Limited compound separation capability)						
Detection Technology	Mass Spectrometry (High fidelity chemical spectrum fingerprint, Figure 1)	High Pressure Mass Spectrometry (Low fidelity chemical spectrum fingerprint, Figure 1)						
Mass Spectrometer	Linear quadrupole mass filter	3D quadrupole Micro Ion Trap						
Mass Scan Range	15-515 AMU	50-500 AMU						
Library Entries	270,000+ chemical compounds including CWAs, explosives, precursors TICs, TIMs, & narcotics. Onboard libraries include the spectral library as well as Nonproprietary libraries (NIST/EPA/NIH and SWGDRUG mass spectral library).	161 chemical compounds including CWAs, explosives, narcotics, TICs & TIMs. The onboard library is propriety and limited to the device technology.						
Average Analysis Time	4 mins 48 secs (Does not include blank run)	3 mins 53 secs (Does not include blank run, additional clean cycles or possible MS Core replacement)						
Decontamination/ Certification	IP-65-rated enclosure (Protected against dust., Protected against low pressure jets of water from all directions, limited ingress permitted.)	IP-54-rated enclosure (Protected against dust limited ingress, no harmful deposits., Protected against water splashed from all directions, limited ingress permitted.)						
Operating Temperature	0 to 40 °C (32 to 104 °F); <95% relative humidity	0 to 40 °C (32 to 104 °F); <95% relative humidity						
Battery and Power Supply	100-240V 50-60Hz (220 W max); 19V (DC); 2 x #2590 @ 15V Li Ion hot swappable batteries (4 included)	100-240V 50-60Hz; 2 x 7.2V Li Ion hot swappable batteries (4 included)						
Size	33.7 x 33.7 x 40 cm (13.25 x 13.25 x 15.75 in)	29.8 x 21.6 x 12.2 cm (11.7 x 8.5 x 4.8 in)						
Weight	16.3 kg (36 lbs)	4.3 kg (9.5 lbs)						
Graphical User Interface	9" Touchscreen Color Display	5" Color Display						
Communication and Data Export:	2 x USB2.0. Bluetooth, Wi-Fi, Ethernet via USB, integrated GPS	2 x USB2.0, Bluetooth						
Alarm	Visual and/or Audible	Visual and/or Audible						

### **General Procedures:**

The following subsections describe sample preparation and analysis procedures executed by the evaluation team during this comparison study. All sample preparation and analysis were performed following all manufacturer's recommended procedures and guidelines for both devices.

#### Solution and Sample Preparation Section:

### A. Specificity and Sensitivity

- For this area of the comparison study, a 10 mL (1 mg/mL) stock solution was prepared for each individual analyte listed in Table A1 of Appendix A, if required. Isotonitazene and all the explosives were purchased as a reference standard in 1 mg/mL solutions. The exception to this concentration was the TATP standard, which was purchased at a concentration of 0.1 mg/mL. After preparation and transfer to labeled 4 mL vials, the solutions were stored at refrigerated temperatures until use.
- Using the previously prepared stock solutions from step 1 above, a dilution factor of 1:1 was performed using methanol for drugs and acetonitrile:methanol (1:1) solution for explosives to achieve a concentration of 0.5 mg/mL. These were prepared and stored in labeled 4 mL vials and refrigerated until needed.
- 3. Except for the explosive TATP, a 0.1 mg/mL solution was also prepared from each of the 1 mg/mL stock solutions for each analyte listed in Table A1 of Appendix A.

#### B. Inter and Intraday Reproducibility

- 1. To evaluate the inter and intraday reproducibility, a four-component, 200 mg mixture sample was prepared.
  - An analytical balance was used to weigh out approximately 100 mg of Heroin, 80 mg of Quinine, 16 mg of D-Mannitol and 4 mg of Fentanyl. After weighing, each sample was combined into a clean, appropriately labeled 4 mL vial.
  - b. The sample was then vortexed for homogeneity and stored in a secure location until use.

### C. Adjudicated Drug Case Samples/Mock Drug Sample Assessment

- 1. Tablets: one tablet for each of the pertinent drug samples were obtained and placed into their own individual, 2 x 2 inch, labeled Ziploc bag and crushed within the bag using a clean pestle.
- 2. Powders, Crystalline & Plant Material: Approximately 100 mg of sample was weighed out using an analytical balance. After weighing, each sample was carefully transferred to their respectively labeled 4 mL vial and capped.
- 3. The four-component drug mix prepared for the inter and intraday reproducibility sample was used in this area of the assessment as a Mock case sample.

### D. Adjudicated Drug Case Samples/Mock Drug Sample Assessment

- 1. A small portion (approximately BB-sized) of each of the fifteen (15) samples was transferred to a clean weigh boat to avoid contaminating the entire sample. Sample presentation included crushed tablets, crystalline/powder material, and dried plant material.
- 2. Using the manufacturer provided sample preparation kit (See Figure 4), a sterile polyester tipped swab was dipped into a 4mL screw top vial preloaded with ~2mL Methanol.
- 3. The wetted swab was rolled in sample in the weigh boat then placed back into the 4mL vial, broken off at the tip, and the vial was capped and agitated/vortexed for 30 seconds.
- 4. A disposable plastic pipette was used to transfer 2 3 drops from the 4mL concentrated extract vial into a 2mL screw top vial preloaded with ~1mL Methanol to prepare a dilute extract.

#### Analytical Section:

### [Device 1] Analysis Procedure

For each phase of this evaluation, liquid sample extractions in 2mL screw top vials, including solvent blanks of methanol for drugs and equal parts acetonitrile:methanol for explosives, were loaded into a tray rack. An injection sequence was created with the appropriate blank preceding each sample replicate and ran on the same method (see Table 5 for method parameters).

- **Specificity**: Drug Standard, Explosive Trace
- Sensitivity: Drug Trace, Explosive Trace
- Reproducibility: Drug Trace

### [Device 2] Analysis Procedure

After verifying that the trace module was correctly installed and two fully charged batteries were inserted, the device was powered on and a system check was performed using the system check accessory dimethyl phosphonate (DMMP) standard. Once the system check was successfully completed and acceptable, as designated by the on-screen prompt, actual sample analysis was initiated. System checks were performed at the beginning and at least one other time each day.

The on-screen prompts were followed, and a blank, clean trace sampling swab was inserted into the trace module and analyzed. This was done before every analysis to ensure there was no contamination or carryover between samples. Clean cycle(s) and replacement of the core were performed when necessary.

#### **Results and Discussion:**

#### Specificity

Of the single component standard samples analyzed for specificity, only fourteen (14) or 56% were detected with a correct ALARM identification. Nine (9) or 36% of the samples presented a NO TARGET DETECTED, while the remaining two (2) or 8% of the samples prompted the user with Multiple Possible ALARMS. All three (3) replicates of the pseudoephedrine sample were identified as pseudoephedrine as well as for Methamphetamine and/or Cathinone. [Device 2] does have a limited library of only 161 compounds and if eight (8) out of the twenty-five (25) samples tested are removed to accommodate for this library limitation, the device would have scored an 82.4% for correct identification.

#	Chemical	Replicate 1	Replicate 2	Replicate 3	Total Points Available	Detected w/ ALARM	Detected w/Suspect	Multiple Possible Alarms	Misidentification	No Target Detected	Total Correct ID%
1	d-Amphetamine HCI				3	3					100.0%
2	d-Methamphetamine HCI				3	3					100.0%
3	Alprazolam*				3					3	0.0%
4	Caffeine				3	3					100.0%
5	Benzocaine*				3					3	0.0%
6	Quinine*				3					3	0.0%
7	Ketamine HCI				3	3					100.0%
8	Acetaminophen				3	3					100.0%
9	d,I-3,4-MDMA HCI				3	3					100.0%
10	Cocaine HCI				3	3					100.0%
11	Heroin HCI				3	3					100.0%
12	Fentanyl				3	3					100.0%
13	Furanyl Fentanyl				3			3			0.0%
14	Buprenorphine*				3					3	0.0%
15	Oxycodone HCI				3	3					100.0%
16	Tramadol HCI*				3					3	0.0%
17	Pseudoephedrine HCI				3			3			0.0%
18	Clonazepam*				3					3	0.0%
19	Hydrocodone HCI				3	3					100.0%
20	Isotonitazene*				3					3	0.0%
21	ТАТР				3					3	0.0%
22	TNT				3	3					100.0%
23	NB*				3					3	0.0%
24	PETN				3	3					100.0%
25	RDX				3	3					100.0%

Table 5: [Device 2] Results Single-Component Specificity

\*Indicates that the compound is not in the [Device 2] limited library.

For the [Device 1] specificity portion of the study, solutions of the single component analytes were prepared at 1mg/mL in methanol for drugs and 0.1mg/mL in a 1:1 mix of methanol:acetonitrile for explosives. Samples were introduced to [Device 1] by injection of 1µL and ran on the manufacturer's preloaded methods. Out of twenty (20) drugs analyzed in triplicate, fourteen (14) were correctly identified each time by the method's programmed automatic threat flagging (green color code). When including manual data interpretation by the user targeting peaks and searching the libraries (yellow color code), correct identification increases to 54 of 60 drug replicates (90%). Buprenorphine and Isotonitazene eluted late in the run and their peaks did not fully resolve, but this could likely be addressed by extending the final hold time slightly. It should be noted that the 1mg/mL concentration was comparatively high based on sensitivity testing performed as part of this evaluation, and this resulted in a few instances of carryover and peak tailing. A penalty was applied during scoring when a false positive was co-detected with the expected analyte, which occurred in 5 of 75 replicates (6.7%). For example, Pseudoephedrine was detected in each of three replicates, but the user was also presented with a false positive identification of a Methamphetamine analog. No penalty was applied for breakdown compounds or carryover which could be accounted for by sequence of injections. For explosives specificity, TATP, TNT, and Nitrobenzene were all correctly identified automatically in each instance while PETN and RDX were not detected at 0.1mg/mL. Each of the 25 compounds were present in at least one of the libraries, and the average correct detection score (Automatic + Manual) was 84.0%.

#	Chemical	Replicate 1	Replicate 2	Replicate 3	Total Points Available	Correct ID Auto	Correct ID Manual	Misidentification	No Target Detected	Total Correct ID %
1	d-Amphetamine HCl		*		3	3				100.0%
2	(+) or d-Methamphetamine HCl	*			3	3				100.0%
3	Alprazolam				3	3	-			100.0%
4	Caffeine				3	3				100.0%
5	Benzocaine		‡		3	2		1		66.7%
6	Quinine				3	2	1			100.0%
7	Ketamine HCl				3	3				100.0%
8	Acetaminophen				3	3				100.0%
9	d,I-3,4-MDMA HCl	+	*	* ‡	3	2		1		66.7%
10	Cocaine HCl				3	3				100.0%
11	Heroin HCl				3	3				100.0%
12	Fentanyl				3	3				100.0%
13	Furanyl Fentanyl				3	3				100.0%
14	Buprenorphine				3	2			1	66.7%
15	Oxycodone HCl				3	3				100.0%
16	Tramadol HCl				3	3				100.0%
17	Pseudoephedrine HCl	\$	+	+	3			3		0.0%
18	Clonazepam				3	3				100.0%
19	Hydrocodone HCl				3	3				100.0%
20	Isotonitazene	+			3		3			100.0%
21	ТАТР				3	3				100.0%
22	TNT				3	3				100.0%
23	NB				3	3				100.0%
24	PETN				3				3	0.0%
25	RDX				3				3	0.0%

### Table 6: [Device 1] Results Single-Component Specificity

\*Co-detection with breakdown product of expected analyte or minor peak without significance †Carryover from previous sample injection

**‡**Co-detection with False Positive

#### Sensitivity

The limit of detection (LOD) of [Device 2] was determined when either no signal was produced for two (2) or more replicates at a particular concentration; or when three replicates for a concentration produced a Correct ID, Suspect ID and a No Target detected. [Device 2] ranged from > 5  $\mu$ g for TATP down to levels slightly below 0.031  $\mu$ g for both MDMA and RDX. Thirteen (13) out of the fifteen (15) single component compounds or 86.7% of the analytes tested were found to have a LOD between > 0.015  $\mu$ g but  $\leq$  0.5  $\mu$ g. During this area of the study, Furanyl Fentanyl was misidentified as a Heroin ALARM at 0.5  $\mu$ g and at the 2.5  $\mu$ g level this sample gave Multiple Possible ALARMS for both Valeryl Fentanyl and Furanyl Fentanyl.

The limit of detection (LOD) of [Device 1] ranged from  $\geq 0.500 \mu g$  for PETN down to just above 0.0025  $\mu g$  for Ketamine. For drugs, 8 of 10 samples were detected as low as 0.010  $\mu g$ . TATP and TNT were detected down to at least 0.025  $\mu g$ , while RDX was identified by manual data interpretation at 0.100  $\mu g$ , limited to the highest concentration standard available at the time of testing. HMX was run in a 1mg/mL solution, the most concentrated available, but was not detected. All Sensitivity testing was performed in triplicate with methods using 0% initial split, with temperature ramping for their respective samples.

#### Reproducibility

A four (4) component polydrug mixture sample containing 2% Fentanyl, 50% Heroin, 40% Quinine and 8% D-Mannitol was analyzed over a 5-day period to assess intra and inter-day reproducibility. Three (3) replicate samples were analyzed on each day and the results were tabulated accordingly, refer to Table 9. The D-mannitol was used as a distractor within this mixture and was not used for scoring purposes. Over the five (5) days of analysis, [Device 2] presented an overall inter-day detection of 28.9% for the three (3) drug mixture components. The device prompted a correct ALARM or SUSPECT alarm and identification for Heroin for 80.0% or twelve (12) out of the fifteen (15) replicate samples tested. Fentanyl was identified for only one (1) or 6.7% out of the replicate samples tested and the quinine component was not detected in any of the replicate samples.

The same 4-component drug mix used for [Device 2] was analyzed in triplicate on [Device 1] over 5 days to assess reproducibility. The bulk powder sample was extracted in Methanol according to the guidelines in the sample preparation kit included. This extraction was only performed once, with the same vial used for injection across 5 days of data collection. Credit was awarded for correct identification of Heroin, Fentanyl, and Quinine as DMannitol is not readily extractable in organic solvents and thus not detected by [Device1]. Overall detection across the 5 days was 100% for Heroin & Quinine and 73.3% for Fentanyl (11 of 15 replicates). The indeterminate concentration of the extraction and selection of the Trace method with 0% initial split resulted in broad peaks which may have masked low concentration components, i.e. Fentanyl, and affected automatic flagging of Quinine. Even so, the interday correct identification was 91.1%, with 46.7% (21/45) automatically identified and 44.4% (20/45) identified by manual data interpretation.

Day		1			2			3			4			5		Inter-Day Detection
Replicate	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3	
Heroin (50%)																80.0%
Fentanyl (2%)																6.7%
Quinine* (40%)																0.0%
Overall Intra- Day Detection		3.3%	6		2.2%	, D		3.3	%		3.3%			2.2%		28.9%

### Table 9: [Device 2] Results Inter & Intraday Reproducibility

\*Indicates that the compound is not in the limited library.

Table 10: [Device 1] Results Inter & Intraday Repro-
--

Day		1			2			3			4			5		Inter-Day Detection
Replicate	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3	
Heroin (50%)																100.0%
Fentanyl (2%)																73.3%
Quinine (40%)																100.0%
Overall Intra- Day Detection	8	8.9%	%	1	00.0	%	7	7.89	%		100.0	%		88.9%	)	91.1%

#### **Adjudicated Case Samples**

To assess the performance of [Device 2] for its ability to detect and identify illicit drugs in real-world samples, fourteen (14) adjudicated drug case samples and one (1) mock drug case sample were run in duplicate. Cocaine base was not detected in either of the replicate samples, cocaine HCl was only detected with ALARM on one (1) replicate and No Target Detected on the other. The heroin sample was misidentified as an ALARM for cocaine. The average overall correct detection and identification for the fifteen (15) samples was determined to be 34.8%. This percentage goes up to 44.4%, if four (4) of the drug samples tested are removed and one (1) of the cutting agents in the Mock case sample is not counted because they contain compounds that are not in the library.

# Table 11: [Device 2] HPMS Results Adjudicated Drug Case Samples

	De consta	GFJC TS	De all'ante d					
#	Drug Sample	#	Replicate 1	Replicate 2				
	MDMA,	TS-124						
	Methamphetamine,							
1	Methamphetamine, and Caffeine Tablet							

identification was 69.6%. The components not identified were Diazepam 5mg tablets, Stanozolol 2mg tablets, Cocaine base with Procaine crystalline material, Marijuana plant material, and the Hydrocodone 5mg dosage in a combination tablet with 500mg Acetaminophen (automatically identified).

Low dosage of pharmaceuticals and age of samples may have affected detection. Manufacturer guidelines dictate preparing a more concentrated extraction and/or rerunning the samples. Results for the four No Target Detected extractions rerun were marginally better, with indications of some expected components. However, the data did not meet the criteria for positive identification (peak abundance  $3\times$  baseline & match factor  $\geq$  70) and thus scoring was not affected. The concentrated vials from the original extraction were not available to attempt another injection from them.

Drug Sample	GFJC TS #	Replicate 1	Replicate 2	Total Points			Misidentification	No Target	Total Correct ID %
MDMA, Methamphetamine, and Caffeine Tablet	TS-124	MDMA, Caffeine, Procaine*	MDMA, Caffeine, Procaine*	6	3	1		2	66.7%
Diazepam, 5 mg Tablet	TS-020	NTD	NTD	2				2	0.0%
Acetaminophen 300mg/Codeine 30 mg Tablet	TS-156	Acetaminophen, Codeine	Acetaminophen, Codeine	4	4				100.0%
Oxycodone, 5mg Tablet	TS-034	Oxycodone	Oxycodone	2	2				100.0%
Hydrocodone 5mg /Acetaminophen 500mg Tablet	TS-071	Acetaminophen	Acetaminophen	4	2			2	50.0%
MX 908 drug mix (powder) Fentanyl, 2% Heroin, 50%, Quinine 40%, D-Mannitol*, 8%	N/A	Heroin, Fentanyl, Quinine	Heroin, <mark>Fentanyl</mark> , Quinine	6	3	3			100.0%
Heroin (Powder)	TS-138	Heroin	Heroin	2	2				100.0%
Ketamine (Powder)	TS-048	Ketamine	Ketamine	2	2				100.0%
d,I-Amphetamine (Powder)	TS-001	Amphetamine	Amphetamine	2		2			100.0%
Methamphetamine HCI (Crystalline Material)	TS-130	Methamphetamine	Methamphetamine	2	2				100.0%
Cocaine HCI (Powder), Levamisole	TS-087	Cocaine, Levamisole†	Cocaine, Levamisole†	4	4				100.0%
Cocaine base, Procaine (Crystalline Material)	TS-047	NTD	NTD	4				4	0.0%
JWH-019 (Powder)	TS-136	JWH-019	JWH-019	2	2				100.0%

Table 12: [Device 1] Results Adjudicated Drug Case Samples

\*Minor peak, not confirmed present in sample

+Common cutting agent, peak acceptable for identification

# Appendix A

# A. Specificity and Sensitivity Section

 Table A1: List of Drug Standards Tested with Source Information

Analyte(s)	Mass (mg)	Lot	Manufacturer	CAS Number
(+) Amphetamine HCl	10.02	71K1581	Sigma	2706-50-5
(+) Methamphetamine HCl	9.97	SLBT1207	Sigma Life Sciences	51-57-0
Alprazolam	10.07	22K4109	Sigma	28981-97-7
Caffeine	10.05	BCBV8010	Sigma-Aldrich	58-08-2
Benzocaine	10.02	SLBR7521V	Sigma-Aldrich	94-09-7
Quinine	9.97	BCBV3272	Sigma	130-95-0
(±) Ketamine HCl	9.96	SLBR8989V	Sigma	1867-66-9
Acetaminophen	9.96	11K0253	Sigma	103-90-2
(±)-3,4-MDMA HCl	10.01	94.3B10.1	Lipomed	64057-70-1
Cocaine HCl	10.04	SLBQ9338V	Sigma	53-21-4
Heroin HCl	10.03	0559234-6	Cayman	1502-95-0
Fentanyl	9.98	622.2B27.1	Lipomed	437-38-7
Furanyl Fentanyl	10.01	0537068-21	Cayman	101365-56-4
Buprenorphine	9.98	SLCD2510	Lipomed	52485-79-7
Oxycodone	10.03	42K1709	Sigma	76-42-6
Isotonitazene	1 mg/mL	FE04282112	Supelco	14188-81-9
Tramadol HCl	10.04	BCCD2302	Sigma	27203-92-5

#### B. Inter and Intraday Reproducibility

 Table A2: Four Component [Device 2] Drug Mixture and Source Information

		% Sample			
Analyte(s)	Mass (mg)	Composition	Lot	Manufacturer	CAS Number
Fentanyl HCl	4.03 mg	2%	622.2B27.1	Lipomed	437-38-7
Heroin HCl	100.05 mg	50%	29.3B37.1	Lipomed	5893-91-4
Quinine	80.02 mg	40%	BCBV3272	Sigma Life Sciences	130-95-0
D-Mannitol	16.03 mg	8%	WXBC3441V	Sigma- Aldrich	69-65-8

# C. Adjudicated Street Drug Case Assessment

# Table A3: List of Adjudicated Street Drug Case Samples

#	Analyte(s)	Strength T	S #	Form	Shape	Color	Marking	Manufacturer	
1	MDMA, Meth, Caffeine	N/A	124	Tablet	Round	Purple	Angel head	N/A	
2	Diazepam	5 mg	020	Tablet	Round	Orange	Mylan 345	Mylan	
3	Acetaminophen / Codeine	300 mg / 30 mg	156	Tablet	Round	White	3TV150	TEVA USA	
4	Hydrocodone/ Acetaminophen	5 mg / 500 mg	071	Tablet	Oblong	White	M357	TEVA	
5	Oxycodone HCl	5 mg	034	Tablet	Round	White	A, 5	Amide	
6	MX 908 Drug Mix	Refer to A2.							
7	Heroin	N/A	138	Powder	N/A	Brown	N/A	N/A	
8	Ketamine	N/A	048	Powder	N/A	White	N/A	N/A	
9	Amphetamine	N/A	001	Powder	N/A	Off-White	N/A	N/A	
10	Methamphetamine HCl	N/A	130	Crystalline	N/A	Colorless	N/A	N/A	
11	Cocaine HCl	N/A	132	Powder	N/A	White	N/A	N/A	
12	Cocaine Base	N/A	065	Chunky	N/A	Off-White	N/A	N/A	
13	JWH-019	N/A	136	Powder	N/A	White	N/A	N/A	
14	Stanozolol	2 mg	012	Tablet	Round	Pink	53 W	Ovation	
15	Marijuana	N/A	101	Plant	N/A	N/A	N/A	N/A	