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Evaluation of the DeltaNu® ReporteR™ Portable Raman Spectrometer

Project Information

Title: Evaluation of the DeltaNu® ReporteR™ Portable Raman Spectrometer

Evaluation Type: Portable Raman Spectrometer

Stakeholder: DeltaNu, Inc.

Start Date: 05/10/2010 End Date: 07/14/10

Kit Model Number(s): 2.11

Serial Number(s): 701-009

United States List Price: $15,000

Manufacturer Information

Manufacturer:

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Evaluation Overview

The Forensic Services Chemistry Section of the National Forensic Science Technology Center (NFSTC) performed an evaluation of the DeltaNu® ReporteR™ (Version 2.11). This palm-sized Raman spectrometer is

currently used by law enforcement, border patrol officers, military personnel and other first responders to chemically characterize unknown solids, liquids, and powders encountered in field environments. The evaluation included accuracy and reproducibility assessments of conformity, mixture sensitivity, specificity, ruggedness, and portability, including sample preparation and training requirements. The evaluation team also briefly examined the associated NuSpec™ software and its library-building capabilities. The objective of this assessment was to provide data to agencies interested in incorporating portable Raman technology into their laboratory or field-testing protocols.

The instrument was evaluated using samples representative of categories likely to be encountered in a field or first-responder environment, including: controlled substances, common diluents of controlled substances, explosives, common chemicals, and ignitable liquids. In addition, the unit was transported to the Manatee County Sheriff's Office, Forensic Chemistry Laboratory to analyze 20 adjudicated case samples. Each sample was conducted in triplicate, and each of these three trials was performed by a different evaluator.

Product Specifications

The ReporteR weighs approximately 363 grams and is approximately 15.1 cm long (without additional sampling attachment), 3.6 cm deep, and 6.5 cm wide.* The LCD display screen is a window near the top of the unit measuring approximately 3.5 x 1.7 cm. The keypad contains four labeled buttons: a select button (green checkmark), an acquire button (yellow starburst), on/off and cancel button (red circle with a line) and a menu button (blue arrows). When charging, the status "charging" is displayed on the screen whether the instrument is powered on or off, and disappears when the unit is charged. The lithium battery life average is listed at four continuous hours** and time to recharge as approximately two hours. The unit automatically turns off after 30 minutes to conserve the battery's charge. Sampling is performed externally from the instrument via direct contact between neat solids, liquids, or powders with the sampling head or through clear bags, vials, or bottles containing these compounds. Three sampling attachments enable the user to choose the one that is optimal for his needs, including a direct (point-and-shoot) sampling head (PS), a disposable tip right angle attachment (DTRA), and a vial attachment with an 8-mm-vial holder. The PS and DTRA attachments have three focal lengths, marked "i", "ii", and "iii", easily adjusted by twisting for sampling optimization. The ReporteR comes with a wall charger, an accessory car charger, a computer USB charger, an SD card, the NuSpec software with libraries, a polystyrene ASTM standard for performance checks and a rugged carrying case, equipped with safety glasses. The only consumables associated with this unit are optional 8-mm vials.

**Measurements are reported as made by evaluators at NFSTC. The Instruction Manual (p. 6) lists the weight and measurements as slightly different.*

***This was not defined in product literature and not evaluated by NFSTC.*

The ReporteR has a rugged design including a rubberized orange casing with a flip-top enclosure at the bottom, protecting the USB port, SD card, and interlock from environmental conditions. The device is designed to be stored in temperatures from -30 to 60°C and operated in temperatures ranging from -20 to 40°C, at altitudes of up to 3,000 meters. According to the Instruction Manual, the ReporteR should be stored out of direct sunlight and is not waterproof. It is equipped with a class IIIB laser source that operates at 785 nm and from 50 to 120 mW. The reported spectral range of the ReporteR is from 300 to 2000 cm^{-1}, with a 12 to 15 cm^{-1} resolution.

The ReporteR's function is based on Raman spectroscopy, which measures the inelastic scattering of monochromatic laser light by molecules in a sample. The scattered light is collected by optics, separated by a monochromator, and detected with a charge-coupled detector (CCD). The CCD measures the intensity of light at each wavelength and converts it to a spectrum, characteristic of a chemical compound. The spectrum from the sample is then searched against entries in the libraries in the instrument's memory. Match quality is assigned a "correlation match indicator" based on similarity of the sample spectrum to the closest library spectra. This is displayed in bars as follows: 5 bars: 0.95 to 1.00 (highest correlation); 4 bars: 0.90 to 0.94; 3 bars: 0.80 to 0.89; 2 bars: 0.70 to 0.79; 1 bar: 0.60 to 0.69 (lowest correlation). If the correlation falls below the one bar range (less than 0.60), the instrument will display "No Match" and zero bars. In both a "match" and "no match" situation, the top three most highly correlated library entries are listed, in order of highest correlation to lowest.

The ReporteR can be operated when attached to the computer or independently. When operated from the computer, comparison spectra can be viewed. According to the Instruction Manual, the libraries contain approximately 1,350 spectra of compounds, including law enforcement samples, chemicals, and plastics. Additions to the user library must be made by computer operation, and library updates are conducted to the unit through the NuSpec software. Files are stored sequentially by date on a 1-gigabyte micro-SD card in one of three digital formats (.spc, .dnu or .prn.). These can then be uploaded onto a computer for storage, data analysis, or reporting, depending on the format.

References

Koussiafes, Perry M. The Interpretation of Data Generated from Fire Debris Examination: Report Writing and Testimony, Analysis and Interpretation of Fire Scene Evidence; Ed. Jose Almirall and Kenneth Furton; Boca Raton, FL; 2004.

ReporteR Instruction Manual, ReporteR™ NuSpec™ V2, January 2010. DeltaNu Inc. Intevac Photonics, Inc., Copyright© 2002–2009.

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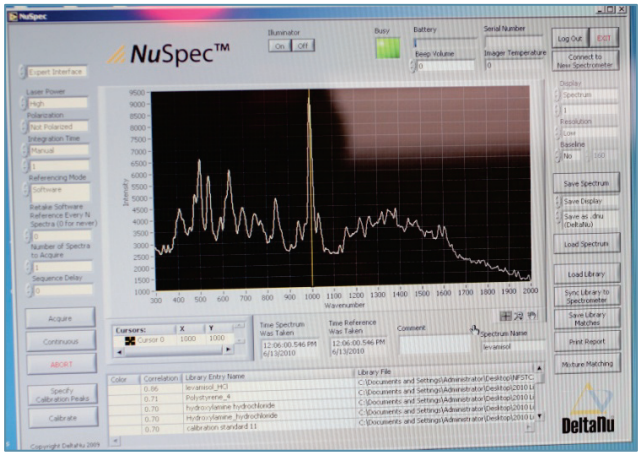
Photos

ReporteR with Kit

ReporteR



NuSpec™ Software Open (levamisole HCl)

Product Uses

The ReporteR can be used to identify a variety of chemical compounds, including a number of drugs (illicit) and pharmaceuticals, explosives, ignitable liquids (or components thereof), oxidizers, and toxic compounds. This function is useful in forensic science applications such as on-target military use, or field use by first responders or law enforcement officers.

Level of Operator Knowledge (Set per Manufacturer)

☒ Non-Scientist ☐ Technician ☐Scientist

Minimal training is required to safely and properly use the instrument and to interpret the results.

Procedure

A total of approximately 111 samples (333 trials) were conducted using the following method for performance checking and sampling:

Calibration

1) Power on the ReporteR by holding down the on/off button for ~1 second.
2) Attach the liquid vial attachment to the ReporteR unit. Place the polystyrene calibration standard into the vial holder.
3) Select the Menu key and select “Self Test”. When prompted by the question “Is the Polystyrene standard loaded?” select start.

4) If the self test passes, proceed to sample analysis. If it fails, re-calibrate the system using the device firmware:
    a. Select Menu and "Re-calibrate".
    b. Select start when prompted by the question "Is the Polystyrene standard loaded?"
    c. If the calibration succeeds, accept and confirm. Continue to sample analysis.
    d. If the calibration fails, proceed to the software installation and calibration steps.

Alternatively:

1) Perform the sample analysis method listed below, using the polystyrene calibration standard against the point-and-shoot (PS) attachment.
2) Record the results; if polystyrene matches with four or five correlation bars, proceed to sample analysis.

Sample Analysis

1) Put on the provided safety glasses.
2) Attach the point-and-shoot (PS) attachment to the unit.
3) Ensure the setting on the PS attachment is set to "iii", the setting recommended by the manufacturer for vials or glass containers (Instruction Manual, p. 12).
4) Hold the side of the sample vial firmly against the PS attachment aperture, ensuring that the contents of the vial are against the glass that is in contact with the aperture.
5) Press the acquire button to turn on the laser and acquire the spectrum. ("Armed" will be displayed on the screen.)
6) Press the select button to display the spectrum, or press the acquire key to display the result.
7) After the spectrum is displayed, press the select button to proceed with a library search.
    a. Match:
        i. Record "Y in the first column.
        ii. Scroll though the matches using the menu button and record, including the number of match quality bars displayed.
        iii. Record "Y" in the "Correct Y/N" column if any of the following criteria are met:
            1. The identity with the largest number of correlation bars matches the identity of the sample;
            2. The identity with the largest number of correlation bars is a synonym for the sample name (e.g., nicotinamide and niacinamide; Tylenol and acetaminophen);
            3. If more than one match out of three has the same largest number of correlation bars and fits the preceding criteria;
            4. If in a mixture, one of the two components was identified with the preceding criteria. *(Note: If in an ignitable liquid mixture, the component must be something that will identify the entire mixture; e.g., "diesel".)*
        iv. Record "N" in the "Correct "Y/N" column if none of the criteria in step "7) a.iii." are met.
    b. No Match:

i. Record “N” in the first column.
ii. Press the select button to read and record the three results. (All entries should have “0” correlation bars.)
iii. Record “N” in the “Correct Y/N” column.

8) Continue by pressing and holding the select button.

Ruggedness Trials

1) Place the ReporteR in the following locations for approximately two hours, performing one trial per day:
    a. **Trial One:** Dashboard of a car;
    b. **Trial Two:** Front seat of a car; and
    c. **Trial Three:** Trunk of a car.
2) Place a portable electronic thermometer at the location with the ReporteR.
3) Record the temperature upon placement and removal.
4) Perform testing as soon as possible using the previously described method.

Library Build Analysis

1) Complete the performance check using the provided reference standard.
2) Scan the following two compounds using the sampling method described to ensure they are not in any of the existing libraries, and record the results:
    a. Papaverine HCl;
    b. Levamisole HCl.
3) Turn on the laptop computer provided with the ReporteR.
4) Attach the ReporteR to the computer using the USB cord.
5) Open the NuSpec software.
6) Open the library build software.
7) Add a new library named “NFSTC”.
8) Ensure that the integration mode is set to “Auto”, “Hardware” mode, “0” for the retake of the software reference, and “Medium” for resolution.
9) Initiate the scan of the two compounds not in the existing library:
    a. Papaverine HCl;
    b. Levamisole HCl.
10) Save the display as a “.dnu” file to the NFSTC library.
11) Load the NFSTC library into the software:
    a. Click “load library”.
    b. Select the NFSTC library and click the “add” button.
12) Sync the NFSTC library to the ReporteR by clicking on the “Sync Library to Spectrometer” button.
13) Sample the two added compounds as described in the sampling method and record results.

Results and Discussion

A total 111 samples* (333 trials) were evaluated using the ReporteR and are listed in the **Appendix, Table 1**. Each sample was analyzed using three trials, and each trial was conducted by a different evaluator at a different time. A performance check was conducted by each evaluator prior to each testing session*.

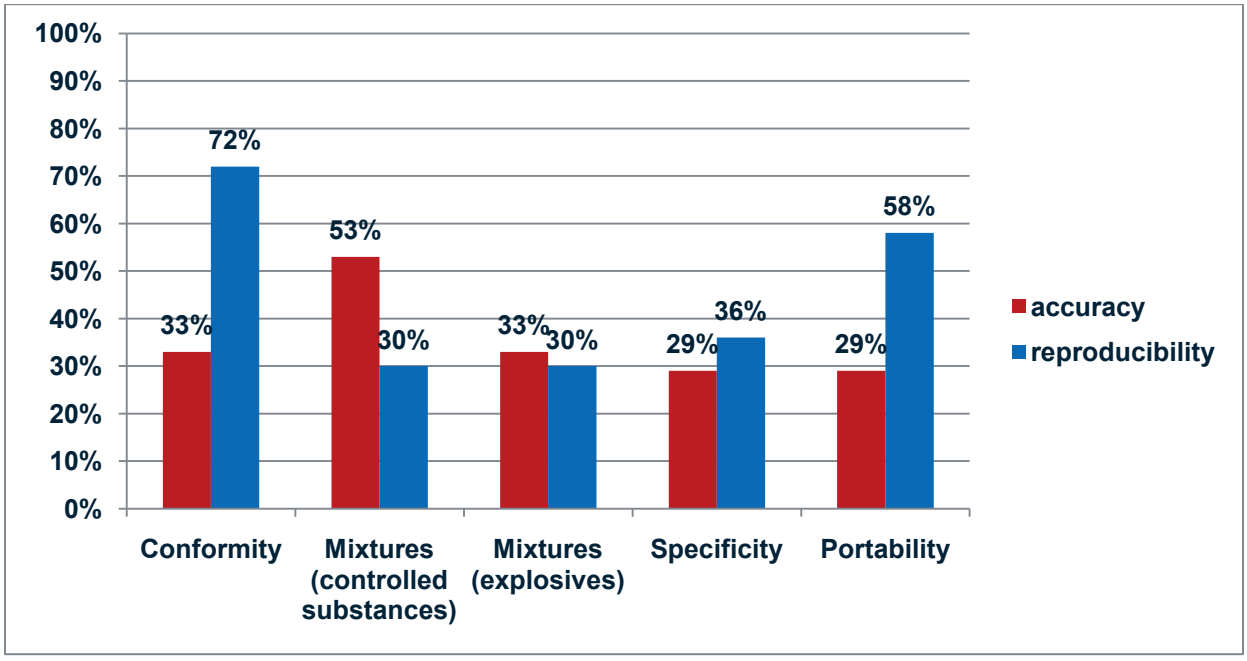
**Performance checks were not included in the sample or trial count.*

Criteria to define accuracy are listed in the described method. (*Note: Because the ignitable liquids in this evaluation are mixtures of many compounds, an accurate answer was defined as one that would enable the user to make an identification. For example, ethanol may be a component of gasoline, but identifying ethanol will not enable a user to identify an unknown liquid as gasoline.*) (See also "Limitations" and "Areas for Improvement".)

Results were defined as reproducible (precise) if the most correlated or equally most correlated (second or third choice as highly correlated as the first) result matched for all three replicates and all were either "matches" or all were "no matches". This included results that were "no match", incorrect matches and synonyms (e.g., sugar and sucrose) in order to correct for a compound not being in the existing libraries. (Note: In "no match" situations, all three results were given equal correlation value.)

Accuracy and reproducibility results for conformity, mixture sensitivity, specificity and portability are summarized in the chart below.

Data Summary for Accuracy and Reproducibility



Conformity Sample Set

Accuracy

Of the 25 samples used to evaluate conformity, the ReporteR accurately identified the target compound in 25 of the 75 trials (~33%). Sixteen of these 75 were controlled substances (methamphetamine, heroin, cocaine HCl) and diluents (caffeine, mannitol, and niacinamide). The remaining nine were explosives (ammonium nitrate and RDX/C-4) and explosive precursors (sugar).

The ReporteR did not accurately identify any of the ignitable liquids tested.

Reproducibility

Eighteen of 25 conformity samples (72%) identified the same most correlated compound (or synonym) for each of three trials. Of these, cocaine HCl, methamphetamine, mannitol, niacinamide, caffeine, sugar, and ammonium nitrate were correctly identified three times each. Of the remaining seven samples, one had three correct most highly correlated results (one with <0.60 correlation), and the other six had two correct results.

Discussion

The ReporteR had better reproducibility between trials than accuracy, as all of the samples had at least two of the same most highly correlated results. Lower accuracy may be due to factors such as inherently weak spectra of certain compounds (e.g., heroin), the nature of the sample (e.g., ignitable liquid) and the exclusion of compounds from existing libraries. Though the ReporteR was unable to identify every controlled substance sample present, it did not incorrectly identify any non-controlled samples tested as controlled substances (no “false positives”).

Notably, the instrument was not able to identify any of the ignitable liquids tested. Some oils and compounds in the library that were frequent matches were specific to brand names. Thus a user would have to be familiar with the specific product to identify the components (hazards, implications, etc.). Because ignitable liquids are mixtures of many compounds, identification may be difficult without mixture-resolving software and/or multiple scans. In addition, identifying a single component of an ignitable liquid mixture would likely not enable the user to make an identification of the liquid mixture. For example, 1-propanol may be a component of lighter fluid, but identifying 1-propanol will not identify an unknown liquid as lighter fluid. (See also “Limitations” and “Areas for Improvement”.)

Mixture Sensitivity Set

Four controlled substances mixture series and two explosive substances series were analyzed in triplicate. Five mixture ratios were prepared by weight of the target compound to the weight of the diluent as follows: 80:20, 60:40, 50:50, 40:60, and 30:70.

Accuracy

Of the four controlled substances mixture series (20 samples with 60 trials), the ReporteR correctly identified one of the two components in 32 of the 60 trials (~53%). Of these, it correctly identified both components in the top three matches once (Cocaine HCl: Caffeine (60:40)). In addition, it distinguished cocaine hydrochloride from cocaine base in all of the cocaine identifications in those mixtures, returning different library entries for each (“cocaine HCL” and “cocaine std” respectively). It did not identify heroin or quinine as a “match” in any of the 15 trials containing these compounds, though “heroine” was listed among the top three results in three “no-match” trials.

The ReporteR identified either ammonium nitrate or sugar in ten of the 15 mixture trials, but identified neither ammonium nitrate nor cumin in any of the 15 trials of that mixture series. Cumin is a common yellow-brown spice that can be used as the fuel in an explosive mixture with ammonium nitrate. Color and fluorescence are two properties known to interfere with Raman spectroscopy.

Reproducibility

Of the four controlled substances mixture series (20 samples, 60 trials), the ReporteR identified the same most highly correlated result for each of three trials half of the time (10 samples, or 30 trials) (50%).

In the explosive substances series, three of ten samples (nine of 30 trials) returned the same most correlated results for all three trials (30%).

Discussion

In three of four controlled substances mixtures, the target compound (drug) was detected reproducibly in the sample with the highest ratio of controlled substance (80:20) and then randomly, if at all, in mixtures of lower ratios. The explosive mixtures were less predictable, as ammonium nitrate was detected throughout the series. An identification trend corresponding to the ratio of components was not observed.

The identification of a component within a (non-liquid) mixture is highly reliant on which component particle of the mixture the Raman laser happens to be fixed. Identifying either component could therefore be considered correct.

Specificity Set

A total of 84 trials were performed on 28 samples to evaluate the ability of the ReporteR to differentiate between compounds similar to common target compounds or commonly associated with target compounds.

Accuracy

In 24 of 84 trials (~29%), the ReporteR accurately identified the target compound. Benzocaine, acetylsalicylic acid (aspirin), ibuprofen (Advil), pseudoephedrine, and acetaminophen (Tylenol), common diluents and OTC drugs, were identified at all trials. Other than one identification of MDA, the ReporteR was unable to identify the phenethylamine group of compounds (MDMA, MDA, and MDEA), as well as diphenhydramine, chlorpheniramine, morphine sulfate, codeine sulfate, lidocaine, and procaine. While it correctly identified urea, it did not properly identify other common chemicals such as sulfuric acid, ammonium hydroxide, and sodium hydroxide. (*Note: Guaifenesin, an expectorant, was identified as "guaiacol glycery" in one trial; this was interpreted by the evaluators as the synonym "guaiacol glyceryl ether".*)

Reproducibility

In 10 of 28 samples (~36%), the results were reproducible across all three trials. Of these, benzocaine, acetylsalicylic acid, ibuprofen, pseudoephedrine, acetaminophen and urea reported three correctly identified "matches" each. Amphetamine and urea each had three correct results, but each had two of these trials listed as "no-match". MDMA had reproducible incorrect identifications (as MDA), but one was listed as a "no-match".

In three additional samples, the most highly correlated match results were the same for two of the trials.

Discussion

Though the results for the phenethylamine compounds (MDEA, MDA, and MDMA) showed little accuracy, they reproducibly resulted in a phenethylamine compound. Since both MDA and MDMA are listed as results, the ability of the ReporteR to differentiate between the two is suspect.

Some compounds such as chlorpheniramine and ferric nitrate resulted in similar but not accurate matches (brompheniramine and calcium nitrate). These results could be due to a lack of reference spectra within the existing libraries or the inability of the software to resolve the differences.

Ruggedness Set

Eight samples were tested using heat to measure the ruggedness of the unit. These trials were intended to model some of the storage and transportation practices by law enforcement officers, first responders, and field users. Samples were chosen to represent different categories of compounds. According to the Instruction Manual (p. 7), the instrument should function at temperatures from -20 to 40°C (-4 to 104°F), and can be stored in temperatures from -30 to 60°C. The unit should not be submersed in water, nor stored in direct sunlight. *(Note: Trials are not listed in chronological order by date performed.)*

Three of the compounds used for this trial were not accurately identified under normal laboratory conditions. For the purposes of the following three samples sets, the "conformity" results were compared to the "ruggedness" results for these compounds (ammonium perchlorate, BP® 87 octane gasoline, and BP® diesel fuel).

Trial One:

The instrument was placed on the dashboard of a car for approximately two hours. The interior temperature upon placement was ~60°C (~141°F). Upon removal, the thermometer's screen was not readable*.

**It is possible that the temperature exceeded the threshold of the thermometer (70°C or ~158°F) and was thus immeasurable.*

Accuracy
The performance check passed and the instrument correctly identified five of the eight target compounds.

Reproducibility
N/A: The conditions were not similar enough after sampling eight samples to perform in triplicate.

Trial Two:

The instrument was placed on the front seat of a car for approximately two hours. The interior temperature upon placement was ~27°C (~81°F). Upon removal, the interior temperature was ~41°C (~106°F).

Accuracy
The performance check passed and the instrument correctly identified eight of the eight target compounds.

Reproducibility
N/A: The conditions were not similar enough after sampling eight samples to perform in triplicate.

Trial Three:

The instrument was placed in the trunk of a car for approximately two hours. The interior temperature of the trunk upon placement was ~36°C (~97°F). Upon removal, the interior temperature was approximately 36°C (~97°F).

Accuracy
Sampling was conducted despite the repeated failure of the ReporteR performance test. It correctly identified six of the eight total target compounds. It also returned a correct "no-match" result for methamphetamine. After testing, attempts were made to cool the unit off and manually recalibrate (using the NuSpec software) without success. The ReporteR did respond to manual calibration later that day and prior to Trial Two.

Reproducibility
N/A: The conditions were not similar enough after sampling eight samples to perform in triplicate.

Discussion

Despite the fact that the temperature neared or exceeded the recommended operating temperature (upper limit) in each of the three trials, the performance of the ReporteR was comparable to that in normal laboratory conditions. Twelve of these 24 trials resulted in an accurate matching most correlated (or equally most correlated) result. Eight more resulted in the same most correlated result as the Conformity Set.

Portability Set

The ReporteR was transported to the Manatee County Sheriff's Office, Forensic Chemistry Laboratory to analyze 20 adjudicated controlled substance case samples. Each sample was tested by three evaluators*. A performance check was performed by each evaluator before proceeding. Samples included six tablets, seven cocaine HCl and base exhibits, five heroin exhibits, and two exhibits in which no controlled substance was detected (lidocaine and presumably acetaminophen). Tablets were crushed and placed into vials before testing.

**One sample, previously identified as cocaine base, was not tested by one evaluator.*

Since Lortab and Darvocet tablets have such a large percentage of acetaminophen, and this substance could help identify a tablet, acetaminophen was defined as a positive identification (accurate response) for these tablets. One sample (presumed acetaminophen) had not been identified by the Sheriff's Office. Results from analyzing the sample were used only for reproducibility.

Accuracy

In total, the ReporteR correctly identified the samples in 16 of 56 trials (~29%).

The ReporteR was able to identify acetaminophen in five of the six trials, the major component of two of the tablets (Darvocet and Lortab). It did not identify the minor component in any of the top three matches in any of the trials. All trials for the alprazolam (Xanax 2 mg), methadone (Methadone 10 mg), and oxycodone (Roxicodone 15 and 30 mg) tablets resulted in "no match".

The ReporteR identified cocaine* as the most correlated match in ten of the 19 total trials (~52.6%) and as the most correlated "no-match" in eight more trials. One returned a "no match, no signal" result. (In error, one trial was not completed.)

**The match of "cocaine std", and "cocaine HCl" was counted as a correct match for both cocaine HCl and cocaine base exhibits.*

Reproducibility

Eleven of the 19 samples (~58%) had reproducible results across the three trials and were either all "matches" or all "no matches". This included one sample in which all evaluators reported "No Match, No Signal" and three samples of heroin in which there were no matches listed but "aniline-2-sulfon" was listed first. Three of the cocaine samples reported cocaine as the mostly highly correlated result for all three trials, but were mixed "match" and "no match" results.

Discussion

The sample set provided to the evaluators included six tablets and one non-controlled, unidentified sample. Each tablet had to be crushed in order to sample it using the same method as the other samples in this evaluation. The presence of an entire crushed tablet in a field-type setting is unlikely. The ability to identify a small amount of a target controlled substance in a tablet is also unlikely. The ReporteR performed especially well with cocaine identification, though the result was not always listed with correlation high enough to be considered a "match". The ReporteR was as accurate and precise on the case samples as on the samples in the laboratory, though its inability to identify heroin could be an issue in jurisdictions where heroin is a problem.

Library Build

Accuracy

Papaverine HCl and levamisole HCl were successfully added to the library and synched to the ReporteR unit and were then correctly identified. Papaverine had a correlation score of 5 bars, with the other two results returning zero bars. Levamisole HCl had a correlation score of 3 bars, and its two other matches had two bars each.

Reproducibility

Papaverine HCl and levamisole HCl were correctly identified after being added to the library.

Discussion

The evaluator was able to build a library, add samples to it, synch it to the instrument, and subsequently identify those compounds through the provided Instruction Manual and trial and error.

Findings

Strengths

- The ReporteR is compact and weighs less than one pound.
- The technique is non-destructive, and little to no sample preparation is required.
- Results are available quickly and in a format understandable to a non-scientist.
- A spectrum is displayed as an option when sampling, which may assist the user in determining the correct positioning between the sample and the sampling tip.
- The three top results are always displayed, even in a "no match" situation.
- The results were highly reproducible, though the correlation scores were not.
- Accuracy could be improved by the user if time is taken to create a user library.

- The unit can operate from -20 to 40°C according to the Instruction Manual, and it operated similarly to normal laboratory conditions even after exposure to temperatures at and above this upper range.
- The unit is easy to operate with a menu-driven user interface.
- Results can be reviewed directly on the device by date.
- Data formats for GRAMS software (.spc) and for Microsoft Excel (.prn) allow users to access files with other programs.
- The battery can be recharged using a wall unit, a car unit, or by attaching the ReporteR to a computer with the USB cord.
- The only consumables for the unit are liquid sampling vials. However, sampling can be done through glass or plastic containers and are thus not often needed, keeping the cost low.
- The cost of the unit is relatively low compared to other portable Raman spectrometers.

Areas for Improvement

- Three results are always displayed, even in "no-match" situations.
    - In some "match" situations, results with zero correlation bars are still listed.
        - Correct "non-matches" were present numerous times throughout the evaluation (i.e. the unit reported "No Match" and the correct compound with zero bars).
        - Dissimilar compounds were listed as correlating.
    - It may be clearer to state only those results that correlate with a minimum of 0.60 or one bar, in both situations where there are other matches and in situations where there are no matches.
- Though the algorithms give a correlation score to aid the user, the sample and library reference spectra cannot be visually compared on the instrument. They also cannot be uploaded to the software and compared afterwards. It would be useful to enable a comparison, especially when results have matches with low correlations.
- There is no way to name spectra prior to sampling, and no identifying information on the handheld device when viewing results. It would be helpful to have a file name to reference.
- The result names are often truncated on the results screen.
- The standard law enforcement library (dated July 2009) used in this evaluation was relatively limited, with approximately 314. Accuracy could be improved by increasing the size of the existing libraries. *(As of the publishing date of this evaluation, the number of spectra in the standard library is approximately 1,124.)*
- When evaluating the use of the ReporteR through the software, an error continued to arise after taking one sample and attempting to take the next. The computer disconnected from the unit and would not reconnect. The ReporteR indicated that the computer and unit were connected but the software did not. The issue was resolved by closing the software and reopening it.
- It would be useful to have the software incorporated onto the unit, instead of separately on the computer.
- The battery charge indicator was inaccurate. The charge lasted far longer than indicated on the screen.
- Library entries, especially for ignitable liquids, were specific to brand names or to specific ignitable mixtures, or a single component of a mixture was often reported as a "match". It may be more informative to report on the nature of the product. For example, instead of "Calcument mineral": the result could read "petroleum based ignitable liquid".

Limitations

- Portable Raman spectroscopy does not work well with trace evidence. A sufficient quantity of the compound of interest must be available for sampling.
- Raman spectroscopy does not work well on highly fluorescent or pigmented items.
- Raman scattering is an inherently weak signal that can be affected by background light, leading to spectra of poor quality.
- The identification of materials is limited to the reference samples contained in the existing library and/or added to the user library.
- Additions to the user libraries cannot be conducted on the instrument.
- The ReporteR does not have built-in mixture deconvoluting software. Therefore, mixtures will not be reported as such.
- Comparison of sample and reference spectra cannot be conducted on the instrument.
- Running a number of samples consecutively using the software caused errors in the software.
- The identification of a compound in a mixture did not necessarily correspond with the compound in the highest ratio in the mixture.
- Proper training must be conducted in order to correctly interpret a match.
- Performance of the instrument depends on the user to get the proper contact between the sample and the tip of the sampling head, and to choose the correct focal length setting.
- Raman scattering is limited to molecules that have a change in polarization potential in regard to distance between nuclei.

Health and Safety Issues

- The unit has a Nominal Ocular Hazard Distance of 36 inches (the distance at which the radiation has decreased to 2 mW/cm^2). The unit should be held at this distance from the eyes, and the included safety goggles should be worn for protection.
- The laser has the ability to explode samples such as black gunpowder. It should not be used to sample dark-colored materials, nor used near bulk materials. Small samples should be isolated for testing.

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APPENDIX

Table 1

Results reported as displayed.

Sample	Trial	Match? Y/N	Primary ID	Correct? Y/N	# bars	Other ID(s)/ Comments	C2/# bars	Other ID(s)/ Comments	C3/# bars
PERFORMANCE CHECK									
5/26/2010	1	Y	Passed						
5/24/2010	2	Y	Polystyrene	Y	5				
5/27/2010	3	Y	Polystyrene	Y	5				
CONFORMITY									
Cocaine HCl	1	Y	Cocaine HCl	Y	2	Cholestyl benzoa	1	cholestyl benzoa	1
	2	Y	Cocaine HCl	Y	3	Cholestyl benzoa	1	cholestyl benzoa	1
	3	Y	Cocaine HCl	Y	4	Benzyl benzoate	2	n-butyl benzoate	2
Cocaine Base	1	N	dichloroacetic a	N	0	aniline-2-sulfon	0	Aniline-2-sulfon	0
	2	N	aniline-2-sulfon	N	0	aniline-2-sulfon	0	dichloroacetic a	0
	3	N	aniline-2-sulfon	N	0	aniline-2-sulfon	0	acridine	0
Methamphetamine	1	Y	Methamphetamine	Y	3	Methamphetamine	3	iso-amyl benzyl	2
	2	Y	Methamphetamine	Y	3	Methamphetamine	3	iso-amyl benzyl	2
	3	Y	Methamphetamine	Y	4	Methamphetamine	3	iso-amyl benzyl	2
Heroin	1	N	Heroine	N	0	2-amino-4,6-dime	0	diazolidinyl ure	0
	2	N	Heroine	N	0	2-amino-4,6-dime	0	diazolidinyl ure	0
	3	Y	Heroine	Y	1	2-amino-4,6-dime	0	diazolidinyl ure	0
Mannitol	1	Y	Mannitol	Y	4	Mannitol bottle	3	d-mannitol	3
	2	Y	Mannitol	Y	4	Mannitol bottle	3	d-mannitol	3
	3	Y	Mannitol	Y	2	d-mannitol	2	d-Mannitol	2
Niacinamide	1	Y	Nicotinamide	Y	5	Ammonium nitrate	3	Ammonium nitrate	3
	2	Y	Nicotinamide	Y	5	Ammonium nitrate	3	ammonium nitrate	3
	3	Y	Nicotinamide	Y	5	Ammonium nitarte	3	ammonium nitrate	3
Boric Acid	1	Y	Ethanol_2	N	3	Ethanol 2	3	Ajidew N-50	3
	2	Y	Ethanol_2	N	3	Ethanol 2	3	Ajidew N-50	3
	3	Y	Ethanol_2	N	3	Ethanol 2	3	Ajidew N-50	3
Inositol	1	N	cystaine dihydr	N	0	D-(+)-gluconic a	0	D-(+)-glucosamin	0
	2	N	D-(+)-gluconic a	N	0	cystamine dihydro	0	1-2benzisothiaz	0
	3	N	D-(+)-gluconic a	N	0	cystamine dihydro	0	D-(+)-glucosamin	0

Sample	Trial	Match? Y/N	Primary ID	Correct? Y/N	# bars	Other ID(s)/ Comments	C2/# bars	Other ID(s)/ Comments	C3/# bars
Caffeine	1	Y	Caffeine	Y	4	caffeine anhydro	4	Caffeine Anhydro	4
	2	Y	Caffeine	Y	4	Caffeine Anhydro	4	Caffeine Anhydro	4
	3	Y	Caffeine	Y	4	caffeine anhydro	4	Caffeine Anhydro	4
Quinine	1	Y	1,1'-bi-2-naptho	N	1	1-methyl napthal	1	2-ethyl-1-napth	1
	2	Y	1,1' -bi-2-naptho	N	1	1-methyl naphtal	0	2-ethyl-1-napth	0
	3	Y	1,1' -bi-2-naptho	N	1	1-methyl naphtal	1	2-ethyl-1-napth	1
RDX	1	Y	Pentaerythritol	Y	3	C4	3	RDX	2
	2	Y	Pentaerythritol	Y	3	C-4	3	RDX	3
	3	Y	Pentaerythritol	N	3	RDX	2	C4	2
Ammonium Nitrate (prills)	1	Y	cesium carbonate	Y	5	Ammonium nitrate	5	ammonium bicarbo	4
	2	Y	Ammonium Nitrate	Y	5	Cesium Carbonate	5	ammonium nitrate	5
	3	Y	cesium carbonate	N	5	Ammonium nitrate	4	ammonium bicarbo	4
Ammonium Perchlorate	1	Y	Sodium chlorate	N	3	Sodium Chlorate	3	ammonium molybda	2
	2	Y	Sodium Chlorate	N	3	Sodium Chlorate	3	Ammonium Molybda	2
	3	Y	Sodium chlorate	N	3	Sodium chlorate	3	glycol formal	2
Sugar	1	Y	Cane Sugar	Y	3	Sucrose	3	sucrose 2	1
	2	Y	Cane Sugar	Y	2	Sucrose	2	Sucrose 2	2
	3	N	Sucrose 2	N	0	Sucrose	0	Cane Sugar	0
Cumin	1	N	aniline-2-sulfon	N	0	aniline-2-sulfon	0	sorbitan monolau	0
	2	N	aniline-2-sulfon	N	0	aniline-2-sulfon	0	dichloroacetic a	0
	3	N	aniline-2-sulfon	N	0	aniline-2-sulfon	0	sorbitan monolau	0
Urea Nitrate	1	Y	sulfamic acid	N	3	potassium carbon	2	barium carbonate	2
	2	Y	Sulfamic Acid	N	3	Barium Carbonate	2	Potassium Carbon	2
	3	Y	sulfamic acid	N	3	potassium carbon	2	1-hexanesulfonic	2
Ammonium Nitrate (powder)	1	Y	cesium carbonate	Y	5	ammonium nitrate	5	ammonium bicarbo	2
	2	Y	Ammonium Nitrate	Y	5	Cesium Carbonate	5	ammonium nitrate	5
	3	Y	cesium carbonate	Y	5	Ammonium nitrate	5	ammonium bicarbo	5
Mineral Spirits	1	Y	1-propanol	N	4	1-propanol	4	PD-23	3
	2	Y	Maxhib AB-600	N	1	Molybdenum IV ox	0	Sodium Bromide	0
	3	Y	1-propanol	N	3	1-propanol	3	PD-23	3
BP® 87 Octane Gasoline	1	Y	benzyl formate	N	3	dibenzylamine	3	butyl benzene	3
	2	Y	Dibenzylamine	N	3	Butyl Benzene	3	Benzyl Formate	3
	3	Y	benzyl formate	N	3	Toluene 3	3	Toluene 3	3

Sample	Trial	Match? Y/N	Primary ID	Correct? Y/N	# bars	Other ID(s)/ Comments	C2/# bars	Other ID(s)/ Comments	C3/# bars
BP® Diesel Fuel	1	Y	Calcumet Mineral	N	3	Calcumet Mineral	3	1-propanol	2
	2	Y	Calcumet Mineral	N	3	Calcumet Mineral	3	1-Propanol	2
	3	Y	Calcumet Mineral	N	3	Calcumet Mineral	3	1-propanol	2
Kerosene	1	Y	Calcumet Mineral	N	4	Calcumet Mineral	4	nujol	4
	2	Y	Maxhib AB-600	N	1	Molybdenum IV ox	0	Sodium Bromide	0
	3	Y	Calcumet Mineral	N	3	Calcumet Mineral	3	nujol	3
Klean Strip® VM&P Naptha Thinner	1	Y	Calcumet Mineral	N	2	Calcumet Mineral	2	PD-23	2
	2	Y	PD 23	N	2	PD-23	2	PD-28	2
	3	Y	Maxhib AB-600	N	1	Molybdenum IV ox	0	cupric acetate	0
Lamplight® Lamp Oil	1	Y	1-propanol	N	4	1-Propanol	4	nujol	4
	2	Y	PD 23	N	4	1-Propanol	4	1-Propanol	4
	3	Y	1-propanol	N	3	1-propanol	3	nujol	3
Ronsonol Lighter Fuel®	1	Y	1-propanol	N	3	1-Propanol	3	PD-23	3
	2	Y	Maxhib AB-600	N	1	Molybdenum IV ox	0	Undecyl Alcohol	0
	3	Y	Maxhib AB-600	N	1	Molybdenum IV ox	1	sodium bromide	0
Kingsford® Charcoal Lighter Fluid	1	Y	1-propanol	N	4	1-Propanol	4	PD23	4
	2	Y	PD23	N	4	PD-23	4	PD-28	4
	3	Y	Maxhib AB-600	N	1	molybdenum IV ox	0	sodiu bromide	0
MIXTURE SENSITIVITY									
Cocaine HCl: Caffeine (80:20)	1	Y	Cocaine HCL	Y	2	Cholestyl Benzoa	0	Cholestyl Benzoa	0
	2	Y	Cocaine HCL	Y	2	Cholestyl Benzoa	0	Cholestyl Benzoa	0
	3	Y	Cocaine HCL	Y	1	bibenzyl	0	Cholestyl Benzoa	0
Cocaine HCl: Caffeine (60:40)	1	Y	Cocaine HCL	Y	2	Cholestyl Benzoa	0	Cholestyl Benzoa	0
	2	Y	Caffeine Anhydro	Y	1	Caffeine Anhydro	1	Cocaine HCL	1
	3	Y	Caffeine	Y	2	Caffeine Anhydro	2	caffeine anhydro	2
Cocaine HCl: Caffeine (50:50)	1	Y	Caffeine	Y	3	caffeine anhydro	3	caffeine anhydro	3
	2	N	3-chloropropioni	N	0	1-(p-bromophenyl	0	3,3-dinitro-2,2	0
	3	Y	Caffeine	Y	3	Caffeine Anhydro	3	caffeine anhydro	3
Cocaine HCl: Caffeine (40:60)	1	Y	Caffeine Anhydro	Y	3	caffeine anhydro	3	caffeine	3
	2	Y	Caffeine Anhydro	Y	3	Caffeine Anhydro	3	Caffeine	3

Sample	Trial	Match? Y/N	Primary ID	Correct? Y/N	# bars	Other ID(s)/ Comments	C2/# bars	Other ID(s)/ Comments	C3/# bars
	3	Y	caffeine	Y	3	Caffeine Anhydro	3	caffeine anhydro	3
Cocaine HCl: Caffeine (30:70)	1	Y	Caffeine Anhydro	Y	4	Caffeine Anhydro	4	caffeine	4
	2	Y	Caffeine Anhydro	Y	3	Caffeine Anhydro	3	Caffeine	3
	3	Y	Caffeine Anhydro	Y	3	Caffeine Anhydro	3	Caffeine	3
Cocaine Base: Caffeine (80:20)	1	N	Cocaine Std	N	0	Caffeine Anhydro	0	Caffeine Anhydro	0
	2	Y	Cocaine Std	Y	2	benzyl benzoate	1	N butyl benzoate	1
	3	Y	Cocaine Std	Y	1	benzyl benzoate	0	Cocaine HCl	0
Cocaine Base: Caffeine (60:40)	1	N	Caffeine	N	0	Caffeine Anhydro	0	Caffeine Anhydro	0
	2	N	Cocaine Std	N	0	Cocaine HCL	0	ABS-b	0
	3	N	Cocaine Std	N	0	Caffeine	0	Caffeine Anhydro	0
Cocaine Base: Caffeine (50:50)	1	Y	Caffeine	Y	4	Caffeine Anhydro	3	Caffeine Anhydro	3
	2	N	Caffeine	N	0	Caffeine Anhydro	0	Caffeine Anhydro	0
	3	Y	Caffeine	Y	3	Caffeine Anhydro	3	Caffeine Anhydro	3
Cocaine Base: Caffeine (40:60)	1	Y	Caffeine	Y	3	Caffeine Anhydro	3	Caffeine Anhydro	3
	2	Y	Caffeine Anhydro	Y	3	Caffeine Anhydro	3	Caffeine Anhydro	3
	3	Y	Caffeine Anhydro	Y	2	Caffeine Anhydro	2	caffeine 2	
Cocaine Base: Caffeine (30:70)	1	Y	Caffeine	Y	3	Caffeine Anhydro	3	caffeine anhydro	3
	2	Y	Caffeine Anhydro	Y	3	Caffeine Anhydro	3	Caffeine	3
	3	Y	Caffeine anhydro	Y	3	caffeine anhydro	3	caffeine	3
Methamphetamine: DMS (80:20)	1	Y	Methamphetamine	Y	3	Methamphetamine	2	Chlorobenzene	2
	2	Y	Methamphetamine	Y	4	Methamphetamine	3	Chlorobenzene	3
	3	Y	Methamphetamine	Y	3	Methamphetamine	3	Chlorobenzene	2
Methamphetamine: DMS (60:40)	1	Y	Methylsulfoxide	Y	3	DMSO2 Sigma	3	Methysulfone ald	3
	2	Y	Methylsulfoxide	N	3	DMSO2 Sigma	3	Methylsulfone ald	2
	3	Y	Methylsulfoxide	N	2	DMSO2 sigma	2	Methylsuflone ald	2
Methamphetamine: DMS (50:50)	1	Y	Chlorobenzene	N	2	Methampthetamine	1	1,3-diethyl-1,3	1
	2	Y	Methylsulfoxide	N	3	Dichloramethane	2	DMSO2 Sigma	2
	3	Y	Methylsulfoxide	N	2	1,3-dimethyl-1,3-	2	DMSO2 Sigma	1
Methamphetamine: DMS (40:60)	1	Y	Methylsulfoxide	N	3	DMSO2 Sigma	2	Methylsulfone ald	2

Sample	Trial	Match? Y/N	Primary ID	Correct? Y/N	# bars	Other ID(s)/ Comments	C2/# bars	Other ID(s)/ Comments	C3/# bars
	2	Y	Methylsulfoxide	N	1	DMSO2 Sigma	0	Methylsulfone Ald	0
	3	Y	Methamphetamine	Y	2	Methamphetamine	2	1,3-diethyl-1,3	1
Methamphetamine: DMS (30:70)	1	Y	Methylsulfoxide	N	4	DMSO2	3	Methysulfone ald	3
	2	Y	Dichloromethane	N	3	Methyl Sulfoxide	3	Methylsulfone ald	3
	3	Y	Methylsulfone	Y	4	DMSO2 sigma	4	Methylsulfoxide	4
Heroin: Quinine (80:20)	1	N	Heroine	N	0	dichloracetic a	0	Aniline-2-Sulfon	0
	2	N	Dichloroacetic a	N	0	N Phenyl 1 napth	0	Coco Imidazole D	0
	3	N	Heroine	N	0	dichloroacetic a	0	coco imidazole	0
Heroin: Quinine (60:40)	1	N	1,1'-bi-2-naptho	N	0	1-methylnaphthal	0	2-ethyl-1-naphth	0
	2	N	1,1'-bi-2-naptho	N	0	1-methylnaphthal	0	2-ethyl-1-naphth	0
	3	N	Heroine	N	0	2,2-biquinoline	0	1,1-bi-2-naptho	0
Heroin: Quinine (50:50)	1	N	3-chloropropioni	N	0	4-chloro-phthali	0	N,N-diallyl-acet	0
	2	Y	1-(p-bromophenyl)	N	1	3,3' dinitro 2,2	1	4-chloro-phthali	0
	3	N	aniline-2-sulfon	N	0	Aniline-2- Sulfon	0	N-phenyl-1-napth	0
Heroin: Quinine (40:60)	1	N	N-Phenyl-1-napht	N	0	dichloroacetic a	0	aniline-2-sulfon	0
	2	N	N-Phenyl-1-napht	N	0	Aniline-2- Sulfon	0	Aniline-2-Sulfon	0
	3	Y	1-(p-bromophenyl)	N	1	3,3-dinitro-2,2	1	benzolalpyrene	1
Heroin: Quinine (30:70)	1	Y	1,1'-bi-2-naptho	N	1	1-methylnaphthal	1	2-ethyl-1-naphth	1
	2	N	1,1'-bi-2-naptho	N	0	1-methylnaphthal	0	2,2 biquinoine	0
	3	N	1-methylphanphthal	N	0	1,1-bi-2-naptho	0	2-ethyl-1-naphtho	0
Ammonium Nitrate: Sugar (80:20)	1	Y	cesium carbonate	Y	5	Ammonium nitrate	5	ammonium bicarbo	5
	2	Y	Ammonium Nitrate	Y	5	Ammonium Nitrate	5	Cesium Carbonate	5
	3	Y	cesium carbonate	Y	5	Ammonium nitrate	5	ammonium bicarbo	5
Ammonium Nitrate: Sugar (60:40)	1	Y	sucrose	Y	3	cane sugar	3	sucrose 2	1
	2	Y	Ammonium Nitrate	Y	4	Ammonium Nitrate	4	Cesium Carbonate	4
	3	Y	cesium carbonate	Y	5	Ammonium nitrate	5	ammonium bicarbo	5
Ammonium Nitrate: Sugar (50:50)	1	Y	Ammonium Nitrate	Y	5	cesium carbonate	5	ammonium nitrate	5
	2	N	Sucrose 2	N	0	Sucrose 2	0	Ammonium Nitrate	0
	3	Y	Cane sugar	Y	4	Cane sugar	3	sucrose 2	1

Sample	Trial	Match? Y/N	Primary ID	Correct? Y/N	# bars	Other ID(s)/ Comments	C2/# bars	Other ID(s)/ Comments	C3/# bars
Ammonium Nitrate: Sugar (40:60)	1	Y	ammonium nitrate	Y	5	cesium carbonate	5	ammonium bicarbo	5
	2	Y	Sucrose 2	Y	1	Sucrose 2	1	Methyl Acetate	0
	3	Y	Sucrose	Y	4	cane sugar	3	sucrose 2	1
Ammonium Nitrate: Sugar (30:70)	1	Y	sucrose	Y	1	cane sugar	1	disodium monplau	1
	2	N	Hydroxy acetoph	N	0	o-dichlorobenzen	0	Ammonium Nitrate	0
	3	Y	Ammonium Nitrate	Y	5	cesium carbonate	5	Ammonium Nitrate	5
Ammonium Nitrate: Cumin (80:20)	1	N	3-chloropropioni	N	1	4-chloro-phthali	1	N,N-diallyl acet	1
	2	N	aniline-2-sulfon	N	0	aniline-2-sulfon	0	Dichloroacetic A	0
	3	N	No Match, No Signal						
Ammonium Nitrate: Cumin (60:40)	1	N	aniline-2-sulfon	N	0	aniline-2-sulfon	0	3-chloropropioni	0
	2	N	aniline-2-sulfon	N	0	aniline-2-sulfon	0	Dichloroacetic A	0
	3	N	aniline-2-sulfon	N	0	aniline-2-sulfon	0	Dichloroacetic A	0
Ammonium Nitrate: Cumin (50:50)	1	Y	aniline-2-sulfon	N	1	aniline-2-sulfon	1	ammonium bicarbo	0
	2	N	Dichloroacetic A	N	0	aniline-2-sulfon	0	aniline-2-sulfon	0
	3	N	No Match, No Signal						
Ammonium Nitrate: Cumin (40:60)	1	N	aniline-2-sulfon	N	0	aniline-2-sulfon	0	sorbitan monolau	0
	2	N	aniline-2-sulfon	N	0	aniline-2-sulfon	0	Dichloroacetic A	0
	3	N	aniline-2-sulfon	N	0	aniline-2-sulfon	0	3-chloropropioni	0
Ammonium Nitrate: Cumin (30:70)	1	N	aniline-2-sulfon	N	0	aniline-2-sulfon	0	sorbitan monolau	0
	2	N	No Match, No Signal						
	3	N	No Match, No Signal						
SPECIFICITY									
d,l-Amphetamine Sulfate	1	Y	Amphetamine sulf	Y	2	Amphetamine	1	ethyl 4-hydroxy b	1
	2	N	Amphetamine Sulf	N	0	Phenylacetyl chl	0	Ylang Ylang	0
	3	N	Amphetamine Sulf	N	0	iso-amyl benzyl	0	amphetamine sulf	0
MDMA	1	Y	MDA	N	2	MDMA	1	pentaerythritol	0
	2	N	Safrole	N	0	MDA	0	2 Propanol 3	0
	3	Y	MDA	N	1	MDMA	0	Trimethylamine	0
MDA	1	Y	MDA	Y	2	MDMA	1	Trimethylamine	0
	2	N	HN1 (Nitrogen Mus)	N	0	Safrole	0	Hydroxya acetophe	0

Sample	Trial	Match? Y/N	Primary ID	Correct? Y/N	# bars	Other ID(s)/ Comments	C2/# bars	Other ID(s)/ Comments	C3/# bars
	3	N	MDA	N	0	hydroxy acetophe	0	2,2-biquinoline	0
MDEA	1	N	MDA	N	0	MDMA	0	safrole	0
	2	N	Safrole	N	0	MDA	0	MDMA	0
	3	N	MDA	N	0	MDMA	0	hydroxyacetophe	0
Morphine Sulfate	1	N	Aniline-2-Sulfon	N	0	Aniline-2-Sulfon	0	4-chlorophthali	0
	2	N	Titanium Dioxide	N	0	Titanium Dioxide	0	Hexanol Chlorid	0
	3	N	Aniline-2-Sulfon	N	0	Aniline-2-Sulfon	0	sorbitan monolau	0
Codeine Sulfate	1	N	hexamethyl phosph	N	0	2-amino-4,6-dime	0	propyl acetate	0
	2	N	Hexanoyl Chlorid	N	0	Titanium Dioxide	0	Titanium Dioxide	0
	3	N	hexamethyl phosph	N	0	2-amino-4,6-dime	0	propyl acetate	0
Benzocaine	1	Y	Benzocaine	Y	5	ethyl 4-aminoben	4	ethyl 4-hydroxy b	2
	2	Y	Benzocaine	Y	4	ethyl 4-aminoben	4	ethyl 4-hydroxy b	2
	3	Y	benzocaine	Y	5	ethyl 4-aminoben	4	ethyl 4-hydroxy b	2
Lidocaine	1	N	1,3-diethyl-1,3-	N	0	1-hydroxycyclohe	0	methylsulfone ald	0
	2	N	Titanium Dioxide	N	0	Titanium Dioxide	0	1,3 diethyl 1,3	0
	3	N	1,3-diethyl-1,3-	N	0	1-hydroxycyclohe	0	4-hydroxy-4-meth	0
Procaine	1	N	4-carboxybenzald	N	0	propyl paraben	0	2,3-butanedione	0
	2	N	4-carboxybenzald	N	0	2,3 butanedione	0	p-cresol	0
	3	N	4-carboxybenzald	N	0	propyl paraben	0	2,3-butanedione	0
Acetylsalicylic Acid (ASA)	1	Y	Aspirin	Y	3	acetylsalicylic	3	o-cresol	0
	2	Y	Aspirin	Y	3	acetylsalicylic	2	o-cresol	0
	3	Y	Aspirin	Y	3	acetylsalicylic	2	o-cresol	0
Ibuprofen	1	Y	Advil	Y	3	bisphenol A	0	bisphenol A	0
	2	Y	Advil	Y	1	1-4 dioxane3	0	bisphenol A	0
	3	Y	Advil	Y	3	bisphenol A	0	bisphenol A	0
Guaifenesin	1	Y	guaiacol glycery	Y	3	methyl cyclohexan	0	2-hydroxy isobuty	0
	2	N	Maxhib AB600	N	0	Sodium Bromide	0	Molybdenum IV ox	
	3	N	guaiacol glycery	N	0	4-bromoveratrole	0	2,2-biquinoline	0
Diphenhydramine	1	Y	Dibenzylamine	N	4	diphenylmethane	4	Calibration Std	4
	2	Y	Dibenzylamine	N	4	Polystyrene4	4	Calibration Std	4
	3	Y	methylphenylace	N	4	diphenyl methane	4	polystyrene	4
Chlorpheniramine	1	N	(+)-brompheniram	N	0	trimethylolpropa	0	poly 12-vinylpyri	0
	2	N	(+)-brompheniram	N	0	Poly2-vinylpyri	0	m chloro aniline	0
	3	N	(+)-brompheniram	N	0	trimethylolpropa	0	allantoin	0
Pseudoephedrine	1	Y	Pseudoephedrine	Y	4	Isopropyl benzyla	4	iso-amyl benzl	3

Sample	Trial	Match? Y/N	Primary ID	Correct? Y/N	# bars	Other ID(s)/ Comments	C2/# bars	Other ID(s)/ Comments	C3/# bars
	2	Y	Pseudoephedrine	Y	4	Isopropyl benzyla	3	Isopropylbenzyle	3
	3	Y	Pseudoephedrine	Y	4	Isopropyl benzyla	4	bibenzyl	3
Dimethyl Sulfone (DMS)	1	Y	methyl sulfoxide	Y	2	DMSO2 sigma	2	methysulfone	2
	2	Y	dichloromethane	N	4	methyl sulfoxide	3	methysulfone ald	3
	3	Y	methyl sulfoxide	N	4	DMSO2 sigma	3	methylsulfone ald	3
Baking Soda	1	Y	sodium bicarbona	Y	4	sodium bicarbona	4	Kathon CG Preser	3
	2	Y	cesium carbonate	N	2	Potassium Nitrate	2	Kathon CG Preser	2
	3	Y	Kathon CG Preser	N	3	manganese nitrat	3	potassium nitrat	3
Acetaminophen (ACE)	1	Y	Tylenol	Y	5	acetaminophen 2	3	acetaminophen 2	3
	2	Y	Tylenol	Y	4	acetaminophen	3	acetaminophen 2	3
	3	Y	Tylenol	Y	5	acetaminophen 2	3	acetaminophen 2	3
Urea	1	Y	Urea	Y	4	Urea	4	diphenyl phosphi	2
	2	Y	Urea	Y	4	Urea	4	diphenyl phosphi	3
	3	Y	Urea	Y	4	Urea	4	diphenyl phosphi	2
Ferric Nitrate	1	Y	Calcium Nitrate	N	5	Calcium Nitrate	5	Manganese Nitrat	4
	2	Y	Calcium Nitrate	N	5	Calcium Nitrate	5	Manganese Nitrate	5
	3	Y	Calcium Nitrate	N	3	Calcium Nitrate	3	Manganese Nitrate	3
Sodium Perborate	1	Y	sodium phosphate	N	2	sodium phosphate	2	sodium dichromat	1
	2	N	Sodium dichromat	N	0	dimethyl methyl	0	Formaldehyde (in	0
	3	N	hydroxy acetophe	N	0	sodium dichromat	0	ethylenediamine t	0
Fertilizer (13% Total N) Prills	1	N	carbazole	N	0	carbazole	0	9,10-diphenylant	0
	2	N	Aniline-2-Sulfon	N	0	Aniline-2-Sulfon	0	dichloroacetic a	0
	3	N	hydroxy acetophe	N	0	2,2-biquinoline	0	2-nitro-p-anisid	0
Fertilizer (13% Total N) – Ground	1	N	aluminum sulfide	N	0	aluminum sulfide	0	sulfur 4	0
	2	N	acetyl chloride	N	0	Acetyl chloride	0	hexanoyl chlorid	0
	3	N	sodium bromide	N	0	aluminum sulfide	0	aluminum sulfide	0
Turmeric: Cardamom (50:50)	1	N	Aniline-2-Sulfon	N	0	Aniline-2-Sulfon	0	sorbitan monolau	0
	2	N	Aniline-2-Sulfon	N	0	Aniline-2-Sulfon	0	dichloroacetic a	0
	3	N	No Match, No Signal						
Sodium Hydroxide (Lye)	1	N	No Match, No Signal						
	2	N	hydroxyacetophe	N	0	molybdenum iv ox	0	5-3 dimethoxy 2	0

Sample	Trial	Match? Y/N	Primary ID	Correct? Y/N	# bars	Other ID(s)/ Comments	C2/# bars	Other ID(s)/ Comments	C3/# bars
	3	N	hydroxyacetaphe	N	0	2,2-biquinoline	0	2-nitro-p-anisid	0
Sulfuric Acid	1	Y	formaldehyde (in	N	3	formaldehyde (in	3	postassium phosph	2
	2	N	sarcosine	N	0	allyl alcohol	0	1-octadecanol	0
	3	Y	formaldehyde	N	3	formaldehyde	3	postassium phosph	0
Ammonium Hydroxide	1	N	No Match, No Signal						
	2	N	1(2-chloroethyl	N	0	carbazole	0	carbazole	0
	3	N	d-galactose	N	0	d-galactose	0	sucrose	0
Citric Acid	1	Y	citric acid	Y	1	citric acid	1	citric acid 3	1
	2	N	citric acid 3	N	0	glycol formal	0	Glycol formal	0
	3	N	citric acid	N	0	glycol formal	0	Glycol formal	0
RUGGEDNESS									
Performance Check									
5/19/2010	1	N	Failed, Failed Recalibration			Recalibrated Manually 5/19/10			
5/21/2010	2	Y	Polystyrene	Y	5				
5/20/2010	3	Y	Polystyrene	Y	5				
Cocaine HCl 5/19/10	1	Y	Cocaine HCl	Y	1	n-butyl benzoate	0	3-methyl-1-phenyl	0
	2	Y	Cocaine HCl	Y	3	chloestyl benzoa	1	cholestyl benzoa	1
	3	Y	Cocaine HCl	Y	3	triphenylphosphi	1	benzyl benzoate	1
Methamphetamine	1	Y	Methamphetamine	Y	2	Methamphetamine	2	Urea	1
	2	Y	Methamphetamine	Y	2	Methamphetamine	2	Urea	
	3	N	Methamphetamine	N	0	Methamphetamine	0	phenylacetyl chl	0
Caffeine	1	Y	Caffeine	Y	3	Potassium tetrab	2	1-bromopropane	2
	2	Y	Caffeine anhydr	Y	4	Caffeine anhydro	4	Caffeine	3
	3	Y	caffeine anhydro	Y	4	Caffeine anhydro	4	Caffeine	4
Ammonium Nitrate (Powder)	1	Y	manganese nitrat	N	4	potassium nitrat	4	Kathon CG Preser	3
	2	Y	Ammonium nitrate	Y	5	Ammonium nitrate	5	ammonium carbonate	5
	3	Y	Ammonium nitrate	Y	5	cesium carbonate	5	ammonium nitrate	4
Ammonium Perchlorate	1	Y	glycol formal	N	3	Glycol formal	3	potassium chlora	2
	2	Y	sodium chlorate	N	3	sodium chlorate	3	ammonium molybda	3
	3	Y	sodium chlorate	N	3	sodium chlorate	3	ammonium molybda	2
RDX	1	Y	Pentaerythritol	N	2	C4	2	paraldehyde	1

Sample	Trial	Match? Y/N	Primary ID	Correct? Y/N	# bars	Other ID(s)/ Comments	C2/# bars	Other ID(s)/ Comments	C3/# bars
	2	Y	Pentaerythritol	Y	2	RDX	2	C4	2
	3	Y	Pentaerythritol	N	3	C4	2	RDX	2
BP 87 Octane Gasoline	1	Y	Cumene	N	2	Cumene	2	diphenyl phosphi	2
	2	Y	dibenzylamine	N	3	xylenes	3	xylenes	3
	3	Y	benzylamine	N	3	toluene	3	toluene	3
BP Diesel Fuel	1	Y	Calcumet Mineral	N	2	Calcumet Mineral	2	nujol	1
	2	Y	Calcumet Mineral	N	3	Calcumet Mineral	3	PD25	2
	3	Y	Calcumet Mineral	N	3	Calcumet Mineral	2	PD25	
PORTABILITY									
Performance Check									
6/4/2010	**1**	Y	Passed						
6/4/2010	**2**	Y	Polystyrene	Y	5				
6/4/2010	**3**	Y	Polystyrene	Y	5				
501: 7.5 mg Hydrocodone/ 500 mg ACE	1	Y	Tylenol	Y	5	Acetaminophen 2	4	Acetaminophen 2	4
501: (Lortab)	2	Y	Tylenol	Y	5	Acetaminophen 2	3	Acetaminophen 2	3
501	3	Y	Tylenol	Y	5	Acetaminophen 2	3	Acetaminophen 2	3
502: 100 mg Propoxyphene/ 650 mg ACE	1	Y	Tylenol	Y	5	Acetaminophen	3	Acetaminophen 2	3
502: (Davocet)	2	Y	Titanium (IV) oxid	Y	2	Veegum Ultra	1	Tylenol	1
502	3	Y	Tylenol	Y	4	Acetaminophen	2	Acetaminophen	3
503: 15 mg Oxycodone HCl	1	N	Lactose	N	0	PVC Rigid	0	Calfax 1GL-35	0
503: (Roxicodone)	2	N	Lactose	N	0	Starch	0	Starch	0
503	3	N	Lactose	N	0	Starch	0	Starch	0
504: 30 mg Oxycodone HCl	1	N	Lactose	N	0	PVC Rigid	0	PVC Flexible	0
504: (Roxicodone)	2	N	PVC Rigid	N	0	Coco Imidazole D	0	Sorbitan Monolau	0
504	3	N	Lactose	N	0	1-(p-bromophenyl	0	3,3'-dinitro-2,2	0
505: Cocaine Base	1	Y	Cocaine std	Y	3	benzyl benzoate	2	n-butyl benzoate	2
505	2	Y	Cocaine std	Y	3	benzyl benzoate	2	n-butyl benzoate	1
505	3	N	sodium bromide	N	0	Maxhib AB-600	0	molybdenum IV ox	0
506: 2 mg Alprazolam (Xanax)	1	N	Coco imidazole D	N	0	Coyote CMC-300	0	4-chlorophthali	0

Sample	Trial	Match? Y/N	Primary ID	Correct? Y/N	# bars	Other ID(s)/ Comments	C2/# bars	Other ID(s)/ Comments	C3/# bars
506	2	N	Coco imidazole D	N	0	Sorbitan Monolau	0	D-maltose monohy	0
506	3	N	Coco imidazole D	N	0	Coyote CMC-300	0	Sorbitan Monolau	0
507: Cocaine Base	1	N	Cocaine std	N	0	1-chloro-3-fluor	0	Cocaine HCl	0
507	2	Y	Cocaine std	Y	2	benzyl benzoate	1	n-butyl benzoate	1
507	3	N	No Match, No Signal	N					
508: Lidocaine	1	N	m-chloroaniline	N	0	3,3-dimethylbuty	0	pyridoxane	0
508	2	N	Pyridoxane hydro	N	0	3,3-dimethylbuty	0	cyclohexylamine	0
508	3	N	Pyridoxane hydro	N	0	n-chloroaniline	0	cyclohexylamine	0
509: 10 mg Methadone HCl	1	N	Lactose	N	0	4-chloro-phthali	0	bis-(m-nitro-di	0
509: (Methadone)	2	N	Lactose	N	0	1-p-bromophenyl	0	3,3'-dinitro-2.2	0
509	3	N	Lactose	N	0	Coyote CMC-300	0	N,N-dialyl-acet	0
510: Cocaine Base	1	Y	Cocaine std	Y	2	benzyl benzoate	2	isopropylbenzla	2
510	2								
510	3	Y	Cocaine std	Y	2	benzyl benzoate	2	n-buytl benzoate	2
511: Heroin	1	N	No Match, No Signal						
511	2	N	No Match, No Signal						
511	3	N	No Match, No Signal						
50: Cocaine HCl	1	Y	Cocaine HCl	Y	2	cholestyl benzoa	1	cholestyl benzoa	1
50	2	N	Cocaine HCl	N	0	1-chloro-3-fluor	0	chlorobenzene	0
50	3	Y	Cocaine HCl	Y	2	benzyl benzoate	1	cholestyl benzoa	1
49B: Cocaine Base	1	N	Cocaine std	N	0	1-chloro-3-fuor	0	n-butylacetanili	0
49B	2	N	Cocaine std	N	0	1-chloro-3-fluor	0	n-butalacetanili	0
49B	3	N	Cocaine std	N	0	cholestyl benzoa	0	cholestyl benzoa	0
44B: Cocaine Base	1	Y	Cocaine std	Y	2	1-chloro-3-fluor	1	isopropyl benzyla	1
44B	2	N	cocaine std	N	0	Isopropyl benzyle	0	benzyl benzoate	0
44B	3	Y	Cocaine std	Y	2	benzyl benzoate	1	Toluene	1
39: Heroin	1	N	anline-2-sulfon	N	0	Aniline-2-sulfon	0	Sorbitan Monolau	0
39	2	N	No Match, No Signal (x2)						
39	3	N	No Match, No Signal						
38: Heroin	1	N	aniline-2-sulfon	N	0	Aniline-2-sulfon	0	Sorbitan Monolau	0
38	2	N	aniline-2-sulfon	N	0	Aniline-2-sulfon	0	Sorbitan Monolau	0
38	3	N	aniline-2-sulfon	N	0	Aniline-2-sulfon	0	Sorbitan Monolau	0
35: Heroin	1	N	aniline-2-sulfon	N	0	Aniline-2-sulfon	0	Sorbitan Monolau	0
35	2	N	aniline-2-sulfon	N	0	Aniline-2-sulfon	0	Sorbitan Monolau	0

Sample	Trial	Match? Y/N	Primary ID	Correct? Y/N	# bars	Other ID(s)/ Comments	C2/# bars	Other ID(s)/ Comments	C3/# bars
35	3	N	aniline-2-sulfon	N	0	Aniline-2-sulfon	0	Sorbitan Monolau	0
34: Heroin	1	N	anline-2-sulfon	N	0	Aniline-2-sulfon	0	dichloroacetic a	0
34	2	N	aniline-2-sulfon	N	0	Aniline-2-sulfon	0	Sorbitan Monolau	0
34	3	N	aniline-2-sulfon	N	0	Aniline-2-sulfon	0	Sorbitan Monolau	0
10: Cocaine Base	1	Y	Cocaine HCl	Y	2	cholestyl benzoa	0	Cholestyl benzoa	0
10	2	N	Cocaine HCl	N	0	1-chloro-3-fluor	0	trimehtylolpropa	0
10	3	N	Cocaine HCl	N	0	Pseudoephedrine	0	cholestyl benzoa	0
9: NCSD, Fake Cocaine Base	1	Y	Tylenol		4	acetaminophen 2	3	Acetaminophen	3
9	2	Y	Tylenol		2	acetaminophen 2	1	Acetaminophen	1
9	3	Y	Tylenol		3	acetaminophen	2	Acetaminophen	2