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Evaluation of the Smiths Detection RespondeR™ RCI Raman Spectrometer

Project Information

Title: Evaluation of the Smiths Detection RespondeR™ RCI Raman Spectrometer

Evaluation Type: Portable Raman Spectrometer

Stakeholder: Smiths Detection

Start Date: 05/10/2010 End Date: 09/01/10

Kit Model Number(s): 024-1001

Serial Number(s): 502601108E

Cost: $30,000 standard

Manufacturer Information

Manufacturer: Smiths Detection

Phone Number: (203) 207-9700

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Evaluation Summary

The Forensic Services Chemistry Section of the National Forensic Science Technology Center (NFSTC) performed an evaluation of the Smiths Detection RespondeR™ Raman spectrometer. This portable Raman spectrometer is currently used by law enforcement, border patrol officers, military personnel and other first responders to chemically characterize unknown solids, liquids, pastes, gels, and powders encountered in field environments. The evaluation included assessments of conformity, reproducibility, mixture sensitivity, specificity, portability, ruggedness, and ease of use, including sample preparation, library additions and training requirements. The objective of this product assessment was to provide data to agencies interested in incorporating portable Raman technology into their laboratory or field-testing protocols.

The RespondeR 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 analyzed in triplicate, using the vial (internal) sampling method, and each of these three trials was performed by a different evaluator. An abbreviated sample set was then analyzed using the external sampling mode (point and shoot).

Product Specifications

The RespondeR weighs approximately 6.9 pounds out of its Pelican carrying case, without the power cord, and is approximately 8.75" long (not including the external sampling port), 3.88" tall and 7.5" deep. It has a hinged suitcase-like structure, with the sampling ports on the bottom half, a touch screen computer on the upper half, and a handle for carrying when its two latches are closed. The RespondeR comes with a battery charger; a flexible keyboard; an attached stylus for use with the touch screen; a flash drive; a reusable spatula; USB cables for data transfer; a CD-ROM for software upgrade; and a rugged carrying case, equipped with safety glasses. There is a communication compartment on the lower half that contains a USB port, mini-USB port, power cord port, and memory card port which must be closed in wet and hot environmental conditions. If this compartment is closed, the RespondeR unit is advertised to be rugged to rain, sleet, snow, sand storms, and salt fogs. Associated consumables include standard 2-ml gas chromatograph autosampler vials and disposable pipettes (for liquid transfer into vials). Battery life is listed at approximately five hours with a five-hour charge time. According to the *User's Guide*, the RespondeR can be operated in temperatures from -7 to 50°C and stored in temperatures from -20 to 80°C.

The calibration standard is internal and a calibration check is prompted before sampling can begin. If the calibration check fails, the computer prompts for a calibration and advises that it can take three minutes. Sampling is disabled if the subsequent calibration does not pass. Sampling is performed externally (point and shoot) from the instrument using a Class 3B laser on neat samples or through clear bags, vials or bottles in contact with the sampling tip. The sampling tip twists to adjust for optimal focal length. An internal vial mode is also available, which uses a Class 1 laser to sample from as little as 100 micrometers from the bottom of a standard 2-ml gas chromatograph autosampler vial. The user must choose the method (vial or point and shoot) from a menu, as well as the libraries to include in the searches. An intermediate screen demonstrates the initial spectrum created to ensure that the sample is correctly situated. The RespondeR is equipped with a holographic diffraction grating spectrometer and an infrared class 3B laser source (75 mW and 785 nm) with a spectral range from 225 to 2400 cm^{-1} and a resolution of 12 cm^{-1}.

The RespondeR's function is based on Raman spectroscopy, which measures the inelastic scattering of monochromatic laser light by the molecules of a sample. The scattered light is collected by optics and separated by wavelength by a spectrometer. A charge-coupled detector 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 selected by the method and up to ten results are returned. Results are listed with a "Hit Quality" (correlation) score, a decimal number 0–1 based on similarity of the sample spectrum to the closest library spectra, from highest to lowest. The user sets the minimum hit quality score for reporting possible match results. Each spectrum can be immediately compared to the sample spectrum, using any of three views (stacked, overlay, and waterfall). If a mixture is suspected, the user has the option of choosing the best match and performing a search on the residual (subtracted) Raman spectrum. Only the first residual search result is listed in this view, but up to ten can be viewed under the data review screen. Spectra are filed with user-entered "incident" and "sample ID" information, stored on a 2-gigabyte CF card and can be transferred from or

recalled on the instrument. Included libraries are advertised to contain approximately 9,400 entries, and additional libraries can be purchased bringing the total entries to between 14,000 and 15,000.

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.

RespondeR™ System User's Guide, Revision 3, 11/20/2006.

RespondeR RCI™ Raman Chemical Identifier Product Package, Smiths Detection Inc., Revised 9/23/2008, www.smithsdetection.com.

Skoog, D., Holler, F., and Nieman, T. Raman Spectroscopy. *Principles of Instrumental Analysis*; Fifth Edition; USA; 1998.

Photos*

RespondeR operation

RespondeR with Kit

Screen shot

**Photo dimensions were altered to accommodate the report format.*

Product Uses

The RespondeR can be used for qualitative analysis of a variety of chemical compounds, including a number of drugs (illicit) and pharmaceuticals, explosives, components of ignitable liquids, oxidizers, and toxic compounds. Sampling is possible directly on powders, liquids, pastes, solids and gels or through clear bottles or bags containing them. This function provides quick identification of unknowns for 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

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

Procedure

The following method was used for performance checking and sampling:

Calibration Check

1) Power on the RespondeR by pressing the green power button in the upper left corner of the unit. A green LED light will turn on.
2) After ~30 to 60 seconds, the screen will turn on, and Windows and the Smiths software will load. When prompted for the password, type "smiths", then use the stylus to select "start."
3) If necessary, clean the sample compartment and/or the external sampling tip with a cotton swab moistened with isopropanol, methanol, ethanol or acetone.
4) Wait 10 to 30 minutes for the unit to warm up.
5) From the "Advanced Features" menu, select "Calibration check." The calibration standard is internal and the check takes approximately one minute.
6) If the check does not fall within ±2 cm^{-1}, a message box will prompt the user to accept further calibration.
7) If the calibration test and/or calibration passes, proceed to sample analysis.
    a. Select "back"
    b. Select "home"
    c. Select "start"

Sample Analysis

1) Select "Advanced Features" from the menu.
2) Select "Method Manager" from the menu.
3) Select the appropriate sampling method:
    a. Select "External Method" (point-and-shoot method) from the menu, then select "select & edit" from the choices below. Ensure that the following settings are selected:
        i. Point & Shoot
        ii. Total Measurement Time (sec): 20
        iii. Threshold at 0.60
        iv. All preloaded libraries are listed in the "Libraries" box
            1. Aldrich Raman.lib
            2. SmithsRamancc.lib
            3. SmithsRamancwa.lib
            4. SmithsRamanExplosives.lib
            5. SmithsRamanForensics.lib

6. SmithsRamanSolvents.lib

b. Select “Vial Method” (internal vial mode) from the menu and select “select & edit” from the choices below. Ensure that the following settings are selected:
   i. Vial
   ii. Total Measurement Time (sec): 20
   iii. Threshold at 0.60
   iv. All preloaded libraries are listed in the “Libraries” box
      1. Aldrich Raman.lib
      2. SmithsRamancc.lib
      3. SmithsRamancwa.lib
      4. SmithsRamanExplosives.lib
      5. SmithsRamanForensics.lib
      6. SmithsRamanSolvents.lib

4) Select “Save.”
5) If using the external method, put on the protective goggles provided with the unit. *(Note: These are unnecessary if using the internal vial mode.)*
6) Select “Start” from the main menu screen.
7) On the sample information screen, enter the folder to which the data is to be saved (“Incident Name”) as your initials, the date, and “ps” for external sampling and “vial” or “vm” for internal vial sampling, such as “HM060310ps.”
8) Enter the name of the sample (“Sample Name”) as the label on the vial.
9) Select “Continue.”
10) Sample:
    a. External:
       i. Hold the vial still in contact with the external sampling accessory, ensuring the opening on the accessory is in contact with an occupied portion of the vial. (For example, if the vial is half-full, ensure it is on the half-full portion.)
       ii. Click “Yes” to accept the warning that laser radiation will be emitted.
    b. Vial (Internal):
       i. Place the vial in the vial holder, ensuring that the bottom of the vial is covered with the material to be tested.
       ii. Close the vial cover.
11) View the preview screen to observe a snapshot of the spectrum to ensure a spectrum is being generated.
12) Select “Continue” to collect spectral data.
13) Record the top three matches, their hit quality values, and the additional number of matches reported on the data chart.
14) Select “Visual Compare.”
15) Report the top three matches, their hit quality values, and the additional number of matches reported in the data chart.

a. Match:
    i. Record “Y” in the “Correct? Y/N” column if any of the following criteria are met:
        1. The identity with the highest hit quality matches the identity of the sample
        2. The identity with the highest hit quality is a synonym for the sample name (e.g., nicotinamide and niacinamide; Tylenol and acetaminophen)
        3. If more than one match out of the possible three has the same hit quality value 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”)
    ii. Record “N” in the “Correct? “Y/N” column if none of the criteria in Step 15) a.i. are met.
b. No Match:
    i. Record “N” in the “Correct? Y/N” column.

16) If indicated by the data sheet, highlight the match with the highest hit quality value and select “Search Residual.”
17) Record the result and the value.
    a. Record “Y” in the “Correct? Y/N” column if any of the criteria in Step 15) a.i. are met by the first residual result.
18) Select “Done” when complete, then select “Home.”

Library Addition

1) Perform the Calibration Check as previously described.
2) Select “Advanced Features.”
3) Select “Method Manager.”
4) Select the “vial method.”
5) Select “select & edit.”
6) Add the user library to the method by selecting “USER.LIB” in the left-hand column and selecting “Add” below the columns.
7) Select “Save.”
8) Select “Done” to exit to the advanced features menu.
9) Select “Home” to exit to the main menu.
10) Analyze the library samples using the previously described vial method:
    a. Papaverine HCl
    b. Levamisole HCl
11) At the result screen, select “Visual Compare.”
12) Select “Add Spectrum.”
13) When a box appears prompting “Added spectrum to library: \Hard Disk\RESPONDER\Library\USER.LIB.” select “OK” in the upper right corner of the box.

14) When it returns to the spectra comparison screen, select “Done.”
15) Run each of the added samples using the previously described sampling method to determine if the samples were added correctly and if the software is recognizing these entries.

Results and Discussion

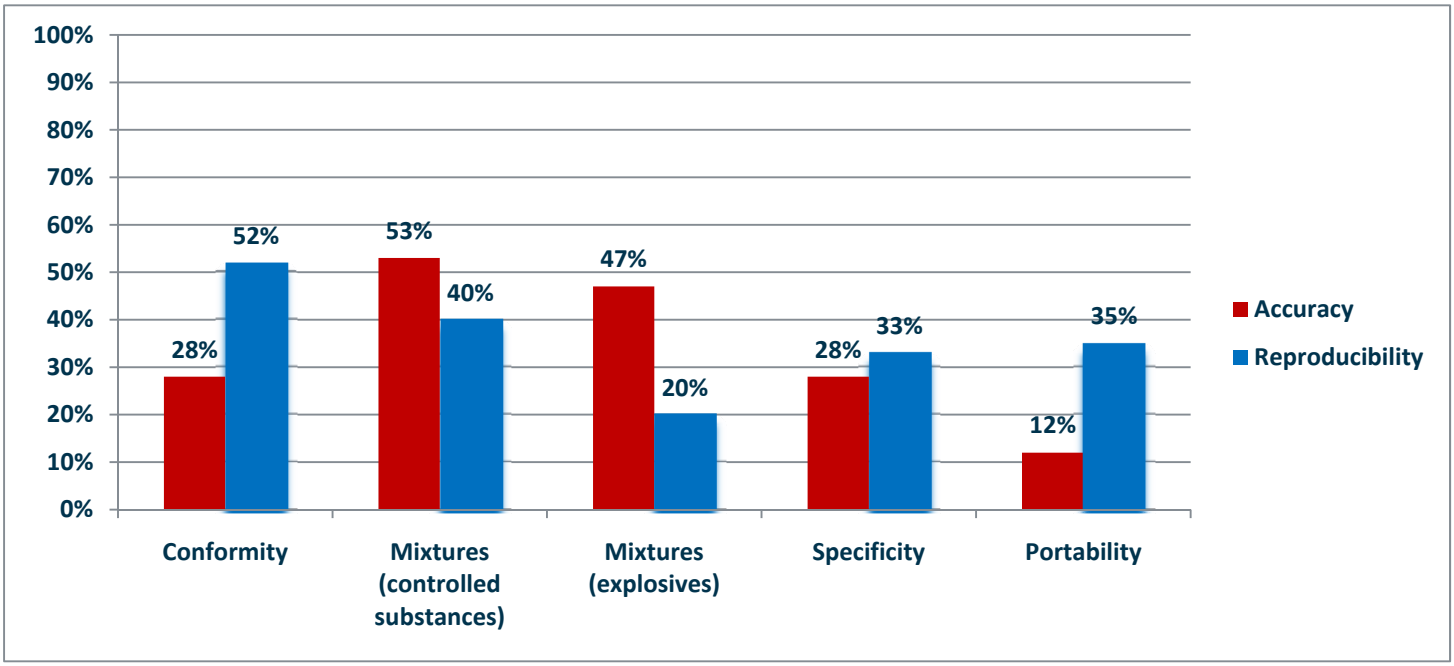
A total of approximately 333 trials were performed using the internal sampling method (“vial mode”) on the RespondeR and are listed in the Appendix, Table 1. Trials using the vial mode were conducted by three different examiners at different times. Due to results during the first trial, evaluation using the external sampling method (“point-and-shoot mode”) was conducted on a more limited scale as shown in the Appendix, Table 2. One full set of conformity, mixture sensitivity, and specificity trials was performed by one evaluator and a representative sampling of each category was performed by a second evaluator. A calibration check* was conducted prior to testing by each examiner, and calibration was performed as needed.

**Calibration checks were not included in the sample/trial count. Sampling cannot commence without a passing calibration check or calibration; therefore, calibration checks are not listed in the data tables.*

Results were defined as reproducible (precise) measurements if the result with the highest hit quality matched for all three replicates. This included results that were “no match” and synonyms (e.g., sugar and sucrose). This was done to correct for a compound not being in the supplied library. Reproducibility will only be discussed for samples analyzed in the vial mode.

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

Data Summary for Sampling in Vial Mode for Accuracy and Reproducibility



Conformity Sample Set

Accuracy

Vial: Of the 25 samples used to evaluated conformity, the RespondeR accurately identified the target compound in 21 of the 75 trials (28%). The following compounds were accurately identified: cocaine (three trials), niacinamide (three trials), boric acid (two trials), caffeine (three trials), RDX (three trials), ammonium nitrate (three trials), sugar (three trials), and VM & P Naphtha Thinner (one trial). If the second and third-listed results are included, then an additional six trials had accurate results (27 of 75 trials, or 36%).

Point-and-Shoot: Ten of 46 trials performed returned an accurate result. Six of these were with the first set of trials, and four were with the second, abbreviated set. If the second and third-listed results are included, then an additional two trials had accurate results (12 of 46 trials, or ~26%).

Reproducibility

Vial: Thirteen of 25 conformity samples (52%) identified the same compound (or synonym) for each of three replicates as the most correlated reference compound. Four of the 13 reproducible results were also accurate.

Point-and-Shoot: N/A

Discussion

The RespondeR had better reproducibility between trials than accuracy. Lower accuracy may be due to a number of factors, including the inherent spectral weakness of certain compounds (e.g., heroin), the nature of the sample (e.g., ignitable liquid) or the exclusion of the sample compounds from existing libraries. In addition, the preliminary spectra displayed before sampling often did not show a strong spectral response. This may have been due to improper focal length, bad contact between the sample and the aperture, or any of the aforementioned factors, or it could be related to other issues such as the detector. The RespondeR repeatedly returned controlled substance results for non-controlled and other controlled substances ("false positives"). For example, butalbital was the second result for two of the caffeine trials and morphine was the second result for two of the niacinamide trials. This type of result could be misleading to a user.

Notably, the instrument was not able to identify most of the ignitable liquids tested. Because ignitable liquids are often mixtures of many compounds, difficulties may arise in identifying them using Raman spectroscopy. The RespondeR also frequently returned brand names, such as "Nujol" (a brand of mineral oil). However, using brand names instead of more general categories (such as "ignitable liquid" or "mineral oil") requires a user to be familiar with the specific product to identify the components (and their properties, hazards, implications, etc.).

Mixture Sensitivity Set

Four controlled substances mixture series and two explosive substances series were analyzed in triplicate using each sampling mode. 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

Vial: Of four controlled substances mixture series (20 samples with 60 trials), the RespondeR correctly identified one of the two components in 32 of the 60 trials (~53%). It did not identify either component in any of the 15 trials of heroin mixed with quinine.

The RespondeR identified either ammonium nitrate or sugar in 13 of the 30 mixture trials (~43%). One of these results was the residual search result. In the mixture series with cumin, ammonium nitrate was only detected once as the result with the highest hit quality and once as the result with the second highest hit quality.

Point-and-Shoot: Of four controlled substances mixture series (20 samples with 28 total trials), the RespondeR correctly identified one of the two components in two of the 28 trials (~7%). It did not identify either component in any of the 15 trials of heroin mixed with quinine.

The RespondeR identified either ammonium nitrate or sugar in two of 14 trials (~14%). It did not return an accurate result for any of the trials of ammonium nitrate and cumin.

Reproducibility

Vial: Of four controlled substances mixture series (20 samples, 60 trials), the RespondeR identified the same component less than half of the time (eight samples, or 24 trials) (40%). In one of the methamphetamine and DMS samples, it identified mescaline as the result with the highest hit quality in three trials. Six of the eight samples identified caffeine as the top result for all three trials and ethidium bromide was the top result (inaccurate) in one sample, for all three trials.

In the explosive substances series, two of ten samples (six of 30 trials), returned the same matches for all three trials (20%). One of these samples included the residual search result (sucrose) as one of the three consistent results.

Point-and-Shoot: N/A

Discussion

Mixture sampling is a well-known limitation of Raman spectrometry. The identification of a component within a (non-liquid) mixture relies heavily on which component particle of the mixture the Raman laser happens to be fixed. Therefore, identifying either component could be considered correct. When a target compound (such as ammonium nitrate) is mixed with a compound that interferes with sampling, the target compound may not be detected at all. Color and fluorescence are two properties known to interfere with Raman spectroscopy. Cumin is a common yellow-brown spice that, among numerous other compounds, can be used as the fuel in an explosive mixture with ammonium nitrate. Ammonium nitrate was detected only once in the mixture series with cumin and cumin was not detected at all.

When probing mixtures, the RespondeR performed more accurately using the vial mode of sampling. The point and shoot mode resulted in only four total accurate identifications overall, none of which were residual searches. Neither sampling method detected methamphetamine, heroin, quinine, cocaine base, or cumin in any of the trials. In addition, both components were not identified in any of the 60 trials and the residual search resulted in only three additional identifications (sucrose in two trials and caffeine in one trial), all in the vial sampling mode. Neither heroin, nor quinine was correctly identified in the conformity trials, so the inability to identify them in a mixture is expected. Caffeine, dimethyl sulfone, and sugar were more often detected than the target compounds in each applicable mixture series, and an identification trend corresponding to the ratio of components was not observed.

Specificity Set

A total of 83* trials were performed on 28 samples to evaluate the ability of the RespondeR to differentiate between compounds similar to common target compounds or commonly associated with target compounds.

**One trial is missing for the vial sampling mode for ibuprofen, so this sample was not used to calculate reproducibility. Each of the two trials resulted in the compound hydroxybutyric acid.*

Accuracy

Vial: In 23 of 83* trials (~28%), the RespondeR accurately identified the target compound. If the second and third highest hit quality results are included, then a total of 28 were accurately identified in the top results. Acetaminophen, aspirin, ibuprofen, benzocaine, guaifenesin, dimethyl sulfone, citric acid, and sulfuric acid were identified at all trials in one of the top three results. It was unable to identify the phenethylamine group of compounds (MDMA, MDA, and MDEA), diphenhydramine, morphine sulfate, codeine sulfate, lidocaine, procaine, and pseudoephedrine, as well as a number of common chemicals.

**One trial is missing for ibuprofen.*

Point-and-Shoot: Six of the 28 trials (~21%) accurately identified the target compound. If the second and third highest hit quality results are included, then an additional sample (ibuprofen) was accurately identified.

Reproducibility

Vial: In nine of 27 samples (~33%), the results were reproducible across all three trials. Of these, six samples reported three correct identifications.

Point-and-Shoot: N/A

Discussion

The RespondeR performed similarly for specificity samples as it did for the conformity set. There were a number of non-controlled substance samples inaccurately identified as a controlled substance as one of the top three results. For example, in two trials, ibuprofen resulted in hydroxybutyric acid (GHB), a Schedule One drug. The mixture samples, such as fertilizer and turmeric–cardamom, did not produce a result that would lead to an identification of the compound. Some compounds such as ferric nitrate resulted in similar but not accurate matches (barium nitrate or chromium nitrate). This could be due to a lack of references in the library or a lack of ability 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 User Manual (p. 19), the instrument should function at temperatures from -7 to 50°C (~19 to 122°F), and can be stored at temperatures from -20 to 80°C (~-4 to 176°F). The unit is reported to be rugged against rain, sleet, snow, sand storms and salt fogs as long as the communication compartment is closed. Ruggedness was tested using the vial mode only.

Four of the compounds used for this trial were not accurately identified under normal laboratory conditions: methamphetamine, ammonium perchlorate, BP® 87 octane gasoline, and BP diesel fuel. For the purposes of the following four samples sets, the conformity results (for at least two of trials) were compared to the ruggedness results for these compounds (mescaline, zinc perchlorate, contact adhesive, and fuel injection cleaner, respectively).

Trial One:

The instrument was placed in the trunk of a car for approximately two hours. The temperature inside the unit upon placement was ~40°C (~105°F). Upon removal, the temperature within the unit was ~42°C (~107°F).

Accuracy
The calibration check initially failed and two calibrations were required for the RespondeR to pass and begin sampling (about 15 minutes after removal). The RespondeR then identified seven 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 dashboard of a car for approximately two hours. The interior temperature upon placement was ~32.5°C (~90.5°F). Upon removal, the thermometer read “HI°C (temperature outside of the unit on the dashboard read 50.0°C). Approximately eight minutes after removal and transport to the air-conditioned laboratory, the temperature read 51.5°C, and after approximately fifteen minutes, it read ~50°C.

Accuracy
The calibration check failed and three subsequent calibrations failed over approximately 15 minutes. This trial was aborted and the instrument was turned off. After warming up the following day, the instrument failed to pass the calibration check and had to be sent to Reachback (support) for repair. A replacement was sent for use during repair (see Trial Three).

Reproducibility
N/A

Trial Three:

The replacement instrument (serial #501511106A) was placed on the front seat of a car for approximately two hours. The interior temperature was ~44.5°C (~112°F) upon removal*.

**Data for temperature upon placement is missing.*

Accuracy
The RespondeR identified four of the eight target compounds

Reproducibility
N/A

Trial Four:

The instrument was placed on the dashboard of a car for approximately two hours. The temperature inside the unit upon placement was ~31.4°C (~88.5°F) and ~63.8°C (~146.8°F) upon removal.

Accuracy
The calibration check failed and the following ten attempts at calibration failed, over approximately 45 minutes (when the temperature read ~40.6°C). This trial was aborted and the instrument was shut down. After warming up, the instrument failed to pass the calibration check the following day.

Reproducibility
N/A

Discussion

In Trials One and Three, the RespondeR performed similarly in heated conditions as it did in laboratory conditions.

The temperature inside of the RespondeR unit exceeded the recommended operating temperature limit of 50°C in two of the trials, though it did not exceed the recommended storage temperature. Even after cooling to temperatures within the recommended operating range, the RespondeR failed calibration and became inoperable for sampling (though review of

results was still possible). It is unknown if the storage temperatures, or the attempts to operate the original and replacement instruments above the recommended operating limits caused the instruments to fail calibration.

Portability

The RespondeR 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 using the vial sampling method. A calibration check and/or calibration were 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.

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

The RespondeR was able to identify acetaminophen in six 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 10mg), and oxycodone (Roxicodone 15 and 30 mg) tablets resulted in inaccurate results. It inaccurately resulted in "ketamine", a scheduled drug, for all three of the lidocaine trials.

The RespondeR identified cocaine* in one of 21 total trials. It did not identify heroin in any of the 15 heroin trials.

**The match of "Icocaine2" was counted as a correct match for both cocaine HCl and cocaine base exhibits.*

Reproducibility

Seven of 20 samples had reproducible results across the three trials. Only two of these samples had three accurate responses (Lortab and Darvocet), each reporting "Tylenol" three times.

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 RespondeR was less accurate on identifying compounds of interest in the case samples than it was on the conformity samples in the laboratory, in which it was able to identify cocaine HCl in three trials. It also inaccurately identified lidocaine as a controlled substance, creating a "false positive" result. Its inability to identify cocaine and heroin in typical "street" samples could hinder its use in jurisdictions where these drugs are a problem.

Library Build

Accuracy

Papaverine HCl and levamisole HCl were successfully added to the user library.

Reproducibility

Papaverine and levamisole HCl were correctly identified, with hit qualities greater than 0.9000 after being added to the library.

Discussion

The evaluator was able to add samples to the user library and subsequently identify those compounds.

Findings

Strengths

- Testing is non-destructive and can be accomplished through sample vials, ensuring the integrity of the evidence.
- A relatively small sample is necessary for vial (internal) sampling. There need only be enough to coat the bottom of the 2-ml gas chromatograph-mass spectrometer (GC-MS) vial. (Photos demonstrate the amounts needed in the *User's Guide*.)
- These vials and caps, as well as disposable pipettes, are the only consumables associated with the RespondeR. These are non-proprietary and can be purchased through numerous vendors.
- Up to ten results are listed as matches, and include their spectra and hit quality scores between zero and one. The user can set the hit quality threshold for returning results.
- There are three different comparisons views: stacked, waterfall, and overlay.
- The software is incorporated into the instrument.
- The calibration standard is internal, and sampling can only continue if the instrument passes the check or calibration, if necessary.
- The calibration check automatically cues the user during extended use.
- There are multiple safety features to protect the user.
- There is a password to access the software to begin sampling, which doubles as a data security feature.
- The laser must be acknowledged before each sample if using the external sampling mode.
- The instrument comes with laser safety goggles.
- There are three warning stickers around the external sampling port.
- Each sample can be given identifying information and saved with a specific "incident", "sample ID" and "comments", prior to sampling.
- Previous results can be displayed and analyzed easily on the device. The aforementioned labeling makes it easy to locate specific spectra.
- The standard library set contains approximately 9,400 spectra, and the expanded library (not part of this evaluation) brings the total to between 14,000 and 15,000.
- The user has the option to perform a residual search on any of the listed matches and can control some of the parameters of this search. Residual searches can be performed when sampling, or later, when recalling data.
- The methods can be edited to tailor the sampling for the user in areas such as sampling time and libraries for comparison.

- The sample vials are standard GC-MS vials, and a limited sample could easily be dissolved and analyzed in the same vial using GC-MS.
- 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 software is easy to operate with a menu-driven user interface.
- Not evaluated:
    - The unit can be linked to the HazmatID using additional software (360 Upgrade) for a more complete chemical analysis.
    - The unit is purported to be waterproof if the communications compartment is closed.
    - Library upgrades are available to increase the size of the libraries.

Areas for Improvement

- The RespondeR needed serviced three times throughout the evaluation. The heat testing caused irresolvable calibration failure twice. The heat trials were designed to mimic storage or transportation practices of a portable-instrument user. Users may not expect the temperature to exceed operating limits within a two-hour period and may not have a thermometer to read the internal temperature of the instrument. Training should emphasize the need for storage, transportation, and use within the specified temperature ranges.
- The unit must be plugged into an outlet to recharge the battery. The ability to exchange dead batteries for charged ones in absence of an electrical outlet would increase its portability.
- The user must go back into the method editor to change from external to vial (internal) sampling, instead of the instrument automatically recognizing the method (for example by the vial compartment door being opened or closed).
- The unit takes 10–30 minutes to warm up prior to sampling. The user's manual lists three different lengths of time for warming up: 10–30 minutes on p. 25, at least 10 minutes on p. 27 and typically 15 minutes on p. 28. Additionally, if the calibration check does not pass, the calibration adds time.
- Sampling takes over a minute, and after each sample, the user must exit to the main screen for information entry.
- The external sampling method displays the current spectra so that the user can maximize the contact and the focal length. However, this feature had a slight time delay that complicated focusing, and the on-screen spectra was poor in most cases. Poor spectra may have been due to factors such as (but not limited to): the time delay, the spectral settings, contact between the aperture and the sample, or aperture size. External sampling would benefit from some adjustments to this feature.
- Files are saved in a proprietary format (.rar), possibly complicating data sharing with users of other instrumentation. These files can only be viewed on the instrument.
- Many of the match names returned with extensive and complicated chemical names. There were links to NIOSH and other information, but the NIOSH information was not loaded, so none of these unknown compounds could be identified in a meaningful way. In addition, the common names were not used for a number of common chemicals. For example, acetaminophen was identified in one instance as "4-acetamidophenol" and benzocaine as "ethyl-p-amino benzoate".
- Library entries, especially for ignitable liquids, were specific to brand names or specific ignitable mixtures. It may be more informative to report on the nature of the product. For example, instead of "Nujol", the result could read "petroleum-based ignitable liquid".

- The residual search resulted in an accurate result (sucrose) in only two trials (cocaine base: caffeine (80:20) and ammonium nitrate: sugar (50:50)), both of which were in vial mode. In most cases, the residual result listed was tetramethylene sulfoxide or terephthalic acid. These were the result with top match quality or the residual search result 54 and 50 times respectively for vial sampling and six and 21 times respectively for point-and-shoot sampling. Neither is a compound with which the evaluators were familiar and neither should have been present in the samples.
- Though technically portable, the RespondeR weighs nearly seven pounds, and cannot be hand-held. This specification limits its use in the field. A lighter weight and/or smaller size could increase its portability.

Limitations

- Raman spectroscopy does not work 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 spectroscopy is an inherently weak signal that can be affected by background light, which leads to Raman spectra of poor quality.
- The identification of materials is limited to the reference samples contained in the library and/or those added to the user libraries.
- This RespondeR does not have built-in mixture deconvoluting software. Therefore, mixtures will not be reported as such.
- Identification of common drugs such as cocaine base, methamphetamine, heroin, morphine and codeine was not accurate or reproducible.
- 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 results.
- 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

Vial Sampling Mode

Results are reported as displayed on the instrument.

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
CONFORMITY									
Cocaine HCl	1	Icocaine2	0.9268	Y	ibuprofen	0.9230	clorazepate	0.8589	7
	2	Icocaine2	0.8924	Y	ibuprofen	0.8865	clorazepate	0.8401	7
	3	Icocaine2	0.8871	Y	ibuprofen	0.8835	clorazepate	0.8602	7
Cocaine base	1	5-isopropyl-m-xylene	0.7403	N	3-bromobenzo-trifluoride	0.7315	triphenyltin fluoride	0.7287	7
Residual	1	tetramethylene sulfoxide	0.6960	N					
	2	5-nitroiso phthalic acid	0.6941	N	5-isopropyl-m-xylene	0.6854	benzyl benzoate	0.6832	7
Residual	2	5-isopropyl-m-xylene	0.6974	N					
	3	3,5 Difluoro nitrobenzene	0.6941	N	3,5-dimethoxy-phenethylamine	0.7566	5-methoxy resorcinol	0.7527	7
Residual	3	phenylboronic acid pinacol ester	0.7210	N					
Methamphetamine	1	mescaline	0.8839	N	(-)ephedrine HCl	0.8268	Valium tab 1	0.8135	6
	2	mescaline	0.8557	N	phenylacetic acid	0.8172	(-)ephedrine HCl	0.8134	6
	3	mescaline	0.7922	N	(1R,2S)-(-)-ephedrine HCl	0.7628	(R)- (+)-3-(Benzyl oxycarbonyl)-4-	0.7547	6
Heroin	1	B-naphthol	0.7611	N	3,4-dinitrotoluene	0.7302	2,4-DNT	0.7020	7
	2	B-naphthol	0.7841	N	3,4-dinitrotoluene	0.7268	ethidium bromide	0.7210	7
	3	B-naphthol	0.8131	N	ethidium bromide	0.7369	3,4-dinitrotoluene	0.7264	7
Mannitol	1	nitroethane	0.8487	N	acetamide	0.8098	D-mannitol	0.8082	4
	2	nitroethane	0.8272	N	acetamide	0.7915	H2O2 30%	0.7832	2
	3	nitroethane	0.8279	N	3-nitro-2-pentanol, mixture	0.7962	2-nitroethanol	0.7887	3
Niacinamide	1	nicotinamide	0.9502	Y	morphine	0.9072	3-picoline	0.8066	4
	2	niacinamide USP	0.9623	Y	morphine	0.9062	K hydrogen phthalate	0.8164	4

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
	3	nicotinamide	0.9536	Y	morphine	0.8977	3-(trifluoro methyl) pyridine	0.8460	3
Boric Acid	1	boric acid 99.5%	0.8749	Y	hydrogen peroxide 30%	0.8494	nitroethane	0.8171	1
	2	boric acid	0.9122	Y	hydrogen peroxide 30%	0.8843	acetamide	0.7685	2
	3	nitroethane	0.8795	N	boric acid 99.5%	0.8509	hydrogen peroxide 30%	0.8331	1
Inositol	1	starch	0.721	N	a-lactose	0.6641	glycogen	0.6639	7
	2	starch	0.7058	N	glycogen	0.6689	a-lactose	0.6669	6
	3	starch	0.707	N	2-chloro-5-nitro benzotrifluoride	0.6805	glycogen	0.6679	7
Caffeine	1	caffeine	0.9056	Y	bromoethane	0.7957	Tetramethyl thiuram disulfide	0.7757	4
	2	caffeine	0.8929	Y	butalbital	0.7550	hexafluoro benzene	0.7504	4
	3	caffeine	0.8753	Y	butalbital	0.7429	Tetramethyl thiuram disulfide	0.7406	3
Quinine	1	1,1-bi-2-naphthol	0.9253	N	ethidium bromide	0.9184	N,N-dimethyl-1-naphthylamine	0.8978	7
	2	ethidium bromide	0.9161	N	1,1-bi-2-napthol	0.9122	Triaminoguanidinium dinitro-pyrazolo-pyrazole	0.9108	7
	3	Hydroquinine	0.9194	N	1,1-bi-2-napthol	0.9160	N,N-dimethyl-1-naphthylamine	0.9148	7
RDX	1	RDX	0.8471	Y	RDX-type 2 class 3	0.7136	boric acid	0.7089	4
Residual	1	tetramethylene sulfoxide	0.7440	N					
	2	RDX	0.8447	Y	RDX-type 2 class 3	0.7577	boric acid	0.6936	5
Residual	2	terephthalic acid	0.7410	N					
	3	RDX	0.8605	Y	nitroethane	0.6454	boric acid	0.6431	5
Residual	3	terephthalic acid	0.7570	N					
Ammonium Nitrate (prills)	1	thallium(ous) nitrate	0.9857	N	ammonium nitrate	0.9782	Mn (II) nitrate tetrahydrate	0.9402	5
	2	ammonium nitrate	0.9818	Y	silver nitrate	0.9749	lead nitrate	0.9694	7
	3	thallium(ous) nitrate	0.9633	N	ammonium nitrate	0.9391	samarium (III) nitrate 6H2O	0.9186	5

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Ammonium Nitrate (powder)	1	ammonium nitrate	0.9816	Y	thallium(ous) nitrate	0.9699	silver nitrate	0.9389	5
	2	ammonium nitrate	0.9794	Y	thallium(ous) nitrate	0.9610	silver nitrate	0.9221	5
	3	thallium(ous) nitrate	0.9761	N	ammonium nitrate	0.9609	Samarium (III) nitrate 6H2O	0.9372	6
Ammonium Perchlorate	1	zinc perchlorate hexahydrate	0.9800	N	cesium perchlorate	0.9796	Mn (II) perchlorate hexahydrate	0.9794	6
	2	cesium perchlorate	0.9834	N	Zinc perchlorate hexahydrate	0.9772	ammonium perchlorate	0.9755	6
	3	zinc perchlorate hexahydrate	0.9819	N	cesium perchlorate	0.9780	Mn (II) perchlorate hexahydrate	0.9719	5
Sugar	1	sucrose	0.8375	Y	Aspartame_Shop Rite Sugar Sub.	0.7819	dextrose anhydride	0.7731	2
	2	table sugar	0.8660	Y	vanilla pudding Jello instant	0.8655	Aspartame_Shop Rite Sugar Sub.	0.8017	2
	3	sucrose	0.8384	Y	Aspartame_Shop Rite Sugar Sub.	0.7851	vanilla pudding Jello instant	0.7509	1
Cumin	1	2,3-dinitrotoluene	0.6058	N	x	x	x	x	0
Residual	1	2,3-dinitrotoluene	0.6060	N					
	2	(Meldola's blue) basic blue 6	0.7328	N	acridine orange channel	0.7221	lanthanum iodide	0.7157	7
Residual	2	(Meldola's blue) basic blue 6	0.7330	N					
	3	tropolone	0.6054	N	2,2':5',2"-terthiophene	0.5701	erythrosin B	0.5627	7
Residual	3	tropolone	0.6050	N					
Urea Nitrate	1	strontium nitrate anhydrous	0.9306	N	zinc nitrate	0.9193	nickel(ous) nitrate	0.9037	6
	2	strontium nitrate	0.9141	N	zinc nitrate	0.8980	sulfamic acid	0.8760	6
	3	potassium nitrate	0.9046	N	cesium hydrogen carbonate	0.8923	strontium nitrate	0.8904	6
Mineral Spirits	1	Nujol	0.9766	N	2-ethylhexyl-amine	0.9480	N,N-dimethyl dodecylamine	0.9416	6
Residual	1	tri-n-butyl citrate	0.7600	N					
	2	Old English lemon oil	0.9558	N	CVS Petroleum Jelly	0.9427	Nujol	0.9426	6
Residual	2	terephthalic acid	0.7220	N					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
	3	Nujol	0.9781	N	europium	0.9623	2-ethylhexyl-amine	0.9544	6
Residual	3	terephthalic acid	0.7510	N					
BP® 87 Octane Gasoline	1	contact adhesive	0.8771	N	lacquer thinner	0.8499	Weld Wood contact cement_dap	0.8264	7
Residual	1	terephthalic acid	0.7560	N					
	2	contact adhesive	0.8907	N	lacquer thinner	0.8552	Weld Wood contact cement_dap	0.8500	7
Residual	2	terephthalic acid	0.7350	N					
	3	contact adhesive	0.8749	N	lacquer thinner	0.8508	Weld Wood contact cement_dap	0.8300	7
Residual	3	terephthalic acid	0.7440	N					
BP® Diesel Fuel	1	fuel injection cleaner Pennzoil Gumont	0.9342	N	Nujol	0.9301	Old English lemon oil	0.9091	6
Residual	1	tri-n-butyl citrate	0.8120	N					
	2	fuel injection cleaner Pennzoil Gumont	0.9243	N	Old English lemon oil	0.9031	ethylene vinyl acetate 50%	0.9022	6
Residual	2	tri-n-butyl citrate	0.7850	N					
	3	Nujol	0.9463	N	fuel injection cleaner Pennzoil Gumont	0.9259	europium	0.9138	6
Residual	3	terephthalic acid	0.7720	N					
Kerosene	1	Nujol	0.9747	N	Old English lemon oil	0.9464	N,N-dimethyl dodecylamine	0.9446	6
Residual	1	tri-n-butyl citrate	0.7920	N					
	2	Nujol	0.9549	N	2-ethylhexyl amine	0.9326	triethylene tetramine	0.9181	6
Residual	2	tri-n-butyl citrate	0.8000	N					
	3	Nujol	0.9819	N	europium	0.9598	2-ethyl hexylamine	0.9499	6
Residual	3	terephthalic acid	0.7720	N					
Klean-Strip® VM&P Naphtha Thinner	1	naphtha VM and P_Klean Strip	0.9412	Y	Nujol	0.9280	Coleman Fuel	0.9125	6
Residual	1	tri-n-butyl citrate	0.7480	N					
	2	Nujol	0.8878	N	dirthromycin	0.8848	2-ethyl hexylamine	0.8802	6
Residual	2	tri-n-butyl citrate	0.7350	N					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
	3	Nujol	0.9318	N	naphtha VM and P_Klean Strip	0.9299	europium	0.9174	5
Residual	3	terephthalic acid	0.7200	N					
Lamplight® lamp oil	1	Nujol	0.9808	N	N,N-dimethyl dodecylamine	0.9477	2-ethyl hexylamine	0.9473	6
Residual	1	tri-n-butyl citrate	0.7830	N					
	2	Nujol	0.9522	N	2-ethyl hexylamine	0.9339	triethylene tetramine	0.9194	6
Residual	2	tri-n-butyl citrate	0.7930	N					
	3	Nujol	0.9846	N	europium	0.9678	2-ethyl hexylamine	0.9554	6
Residual	3	tri-n-butyl citrate	0.7700	N					
Ronsonol lighter fuel®	1	Nujol	0.9646	N	2-ethyl hexylamine	0.9526	naphtha VM and P_Klean Strip	0.9466	6
Residual	1	terephthalic acid	0.7370	N					
	2	2-ethyl hexylamine	0.9262	N	Nujol	0.9232	ligroine	0.9150	6
Residual	2	tri-n-butyl citrate	0.8030	N					
	3	Nujol	0.9630	N	europium	0.9568	2-ethyl hexylamine	0.9559	6
Residual	3	tri-n-butyl citrate	0.7430	N					
Kingsford® charcoal lighter fluid	1	Nujol	0.9820	N	2-ethyl hexylamine	0.9555	N,N-dimethyl dodecylamine	0.9547	6
Residual	1	terephthalic acid	0.7590	N					
	2	Nujol	0.9524	N	2-ethyl hexylamine	0.9378	triethylene tetramine	0.9205	6
Residual	2	tri-n-butyl citrate	0.7820	N					
	3	Nujol	0.9838	N	europium	0.9725	2-ethyl hexylamine	0.9617	6
Residual	3	terephthalic acid	0.7570	N					
MIXTURE SENSITIVITY									
Cocaine HCl: Caffeine (80:20)	1	Icocaine2	0.8268	Y	ibuprofen	0.8217	clorazepate	0.7777	7
Residual	1	tetramethylene sulfoxide	0.7430	N					
	2	Icocaine2	0.8485	Y	clorazepate	0.8485	ibuprofen	0.8432	5
Residual	2	terephthalic acid	0.7555	N					
	3	phenylboronic acid pinacol ester	0.7476	N	Quadra Pure ™ AEA	0.7391	p-dibenzyl oxibenzene	0.7385	7
Residual	3	tri-n-butyl citrate	0.6770	N					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Cocaine HCl: Caffeine (60:40)	1	Icocaine2	0.7330	Y	ibuprofen	0.7279	p-dibenzyl oxibenzene	0.7121	7
Residual	1	tetramethylene sulfoxide	0.7291	N					
	2	caffeine	0.8648	Y	tetramethylthiuram disulfide	0.7704	bromoethane	0.7307	4
Residual	2	tetramethylene sulfoxide	0.7510	N					
	3	Icocaine2	0.7514	Y	ibuprofen	0.7471	clorazepate	0.7419	7
Residual	3	tetramethylene sulfoxide	0.7190	N					
Cocaine HCl: Caffeine (50:50)	1	caffeine	0.8363	Y	butalbital	0.7517	bromoethane	0.6883	4
Residual	1	tetramethylene sulfoxide	0.7240	N					
	2	caffeine	0.8670	Y	tetramethylthiuram disulfide	0.7586	bromoethane	0.7278	4
Residual	2	terephthalic acid	0.7490	N					
	3	caffeine	0.8406	Y	butalbital	0.7381	bromoethane	0.6909	4
Residual	3	tetramethylene sulfoxide	0.7300	N					
Cocaine HCl: Caffeine (40:60)	1	caffeine	0.7862	Y	butalbital	0.6922	3,4-dinitrotoluene	0.6631	4
Residual	1	tetramethylene sulfoxide	0.7130	N					
	2	caffeine	0.8289	Y	tetramethylthiuram disulfide	0.7621	2-chloro-2-methyl butane	0.6863	4
Residual	2	tetramethylene sulfoxide	0.7380	N					
	3	caffeine	0.8822	Y	tetramethylthiuram disulfide	0.7506	bromoethane	0.7432	4
Residual	3	tetramethylene sulfoxide	0.7300	N					
Cocaine HCl: Caffeine (30:70)	1	caffeine	0.9355	Y	butalbital	0.8099	bromoethane	0.7886	4
Residual	1	tetramethylene sulfoxide	0.7420	N					
	2	caffeine	0.8976	Y	bromoethane	0.7829	tetramethylthiuram disulfide	0.7813	4
Residual	2	terephthalic acid	0.7500	N					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
	3	caffeine	0.8138	Y	bis(dimethylthio carbamyl) disulfide	0.7128	Butalbital	0.7017	3
Residual	3	2,3-dinitrotoluene	0.6970	N					
Cocaine base: caffeine (80:20)	1	8-anilo-1-naphthalene	0.6734	N	4-aminoantipyrine	0.6467	L-tryptophan	0.6459	7
Residual	1	tetramethylene sulfoxide	0.7082	N					
	2	caffeine	0.9147	Y	bromoethane	0.8079	tetramethylthiuram disulfide	0.7834	4
Residual	2	terephthalic acid	0.7620	N					
	3	3,5-difluoro nitrobenzene	0.7744	N	b-naphthol	0.6847	8-anilino-1-napthalene-sulfonic acid	0.6832	7
Residual	3	caffeine	0.6820	Y					
Cocaine base: caffeine (60:40)	1	5-nitroisophthalic acid	0.6503	N	3,3 dinitrobenzil	0.6492	8-anilo-1-naphthalene	0.6445	7
Residual	1	p-dibenzyl oxibenzene	0.6580	N					
	2	caffeine	0.8494	Y	tetramethylthiuram disulfide	0.7317	bromoethane	0.7254	4
Residual	2	tetramethylene sulfoxide	0.7230	N					
	3	caffeine	0.8566	Y	butalbital	0.7374	bis(dimethylthio carbamyl) disulfide	0.6711	4
Residual	3	tetramethylene sulfoxide	0.7450	N					
Cocaine base: caffeine (50:50)	1	caffeine	0.8925	Y	butalbital	0.7655	bromoethane	0.7455	4
Residual	1	tetramethylene sulfoxide	0.7450	N					
	2	caffeine	0.7535	Y	tetramethylthiuram disulfide	0.6309	butalbital	0.6213	4
Residual	2	tetramethylene sulfoxide	0.7320	N					
	3	caffeine	0.8970	Y	butalbital	0.7630	bromoethane	0.7618	4
Residual	3	tetramethylene sulfoxide	0.7360	N					
Cocaine base: caffeine (40:60)	1	caffeine	0.8790	Y	butalbital	0.7563	bromoethane	0.7197	4

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Residual	1	tetramethylene sulfoxide	0.7600	N					
	2	caffeine	0.8284	Y	butalbital	0.7047	tetramethylthiuram disulfide	0.6546	5
Residual	2	tetramethylene sulfoxide	0.7300	N					
	3	caffeine	0.8470	Y	butalbital	0.7238	bis(dimethylthiocarbamyl) disulfide	0.6902	4
Residual	3	tetramethylene sulfoxide	0.7160	N					
Cocaine base: caffeine (30:70)	1	caffeine	0.8848	Y	butalbital	0.7649	bromoethane	0.6893	4
Residual	1	tetramethylene sulfoxide	0.7550	N					
	2	caffeine	0.8677	Y	tetramethylthiuram disulfide	0.7297	butalbital	0.6922	4
Residual	2	tetramethylene sulfoxide	0.6840	N					
	3	caffeine	0.8882	Y	bromoethane	0.7534	tetramethylthiuram disulfide	0.7453	4
Residual	3	tetramethylene sulfoxide	0.7270	N					
Methamphetamine: DMS (80:20)	1	mescaline	0.8578	N	(-)ephedrine HCl	0.8208	phenylacetic acid	0.8106	7
Residual	1	terephthalic acid	0.7440	N					
	2	mescaline	0.7857	N	(-)ephedrine HCl	0.7622	Valium tab 1	0.7426	6
Residual	2	terephthalic acid	0.7390	N					
	3	mescaline	0.8268	N	dibenzyl carbonate	0.7869	2,3,4,6-tetra-O-benzyl-alpha-D	0.7853	6
Residual	3	terephthalic acid	0.7470	N					
Methamphetamine: DMS (60:40)	1	methyl sulfone	0.8326	Y	dichloromethane	0.7213	vanadium pentoxide	0.6357	3
Residual	1	terephthalic acid	0.7820	N					
	2	mescaline	0.8566	N	Valium tab1	0.8314	(-)ephedrine	0.8027	7
Residual	2	terephthalic acid	0.7520	N					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
	3	mescaline	0.8363	N	Valium tab1	0.8263	dibenzyl-n,n-diethyl phosphoramidite	0.7965	6
Residual	3	terephthalic acid	0.7510	N					
Methamphetamine: DMS (50:50)	1	methyl sulfone	0.9012	Y	dichloromethane	0.8064	vanadium pentoxide	0.7242	3
Residual	1	terephthalic acid	0.7840	N					
	2	dichloromethane anhydrous	0.7277	N	vanadium pentoxide	0.7069	methyl sulfone	0.6915	3
Residual	2	terephthalic acid	0.7570	N					
	3	(1,1-dimethylpropyl) benzene	0.7619	N	Tert-butylbenzene	0.7567	Valium tab 1	0.7551	7
Residual	3	terephthalic acid	0.7580	N					
Methamphetamine: DMS (40:60)	1	methyl sulfone	0.9510	Y	dichloromethane	0.8591	vanadium pentoxide	0.7442	3
Residual	1	terephthalic acid	0.7800	N					
	2	(1,1-dimethylpropyl) benzene	0.7523	N	1-chloro-2-methyl-2-phenylpropane	0.7146	Valium tab 1	0.7131	6
Residual	2	terephthalic acid	0.7410	N					
	3	(1,1-dimethyl propyl) benzene	0.7036	N	N,N'-diphenyl thiourea	0.6710	Tert-butylbenzene	0.6699	6
Residual	3	terephthalic acid	0.7590	N					
Methamphetamine: DMS (30:70)	1	methyl sulfone	0.7699	Y	vanadium pentoxide	0.7133	1-chloro-2-methyl-2-phenyl propane	0.6968	3
Residual	1	terephthalic acid	0.7690	N					
	2	dichloromethane	0.8315	N	methyl sulfone	0.8039	2,3-dimethyl-2-butanol	0.7300	3
Residual	2	terephthalic acid	0.7480	N					
	3	methyl sulfone	0.9207	Y	dichloromethane	0.8677	2,3-difluorophenol	0.8558	2
Residual	3	terephthalic acid	0.7860	N					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Heroin: Quinine (80:20)	1	B-naphthol	0.7859	N	ethidium bromide	0.7212	acridine orange channel	0.7190	7
Residual	1	3,4-dinitrotoluene	0.7150	N					
	2	ethidium bromide	0.8501	N	B-naphthol	0.8244	triaminoguanidinium dinitropyrazolopyrazole	0.8171	7
Residual	2	3,4-dinitrotoluene	0.7470	N					
	3	ethidium bromide	0.8168	N	B-naphthol	0.7873	hexanitrostilbene (HNS2)	0.7873	7
Residual	3	3,4-dinitrotoluene	0.7230	N					
Heroin: Quinine (60:40)	1	B-naphthol	0.7053	N	poly(vinyl acetate)	0.6713	ethidium bromide	0.6476	7
Residual	1	tetrahydro naphthalene	0.7350	N					
	2	ethidium bromide	0.9092	N	trinitrotoluene (TNT)	0.9020	triaminoguanidinium dinitropyrazolopyrazole	0.9013	7
Residual	2	3-nitro phthalimide	0.7130	N					
	3	ethidium bromide	0.8566	N	triaminoguanidinium dinitropyrazolopyrazole	0.8292	B-naphthol	0.8249	7
Residual	3	3,4-dinitrotoluene	0.7910	N					
Heroin: Quinine (50:50)	1	ethidium bromide	0.8727	N	B-naphthol	0.8486	acridine orange channel	0.8392	7
Residual	1	acridine orange channel	0.8270	N					
	2	ethidium bromide	0.9396	N	trinitrotoluene (TNT)	0.9020	triaminoguanidinium dinitropyrazolopyrazole	0.8928	7

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Residual	2	3-nitro phthalimide	0.7340	N					
	3	ethidium bromide	0.9153	N	triaminoguanidinium dinitropyrazolo pyrazole	0.8852	B-naphthol	0.8823	7
Residual	3	3,4-dinitrotoluene	0.7910	N					
Heroin: Quinine (40:60)	1	ethidium bromide	0.9254	N	B-naphthol	0.9037	triaminoguanidinium dinitropyrazolo pyrazole	0.8794	7
Residual	1	B-naphthol	0.7930	N					
	2	Hexanitrostilbene (HNS2)	0.8240	N	4,6-dinitro-o-cresol	0.7991	2-hydroxy-4-methylquinoline	0.7973	7
Residual	2	4-amino-salicylic acid	0.7912	N					
	3	ethidium bromide	0.9477	N	B-naphthol	0.8627	triaminoguanidinium dinitropyrazolopyrazole	0.8594	7
Residual	3	acridine orange channel	0.8360	N					
Heroin: Quinine (30:70)	1	1,1-bi-2-napthol (sic)	0.9173	N	ethidium bromide	0.9165	triaminoguanidinium dinitropyrazolopyrazole	0.9021	7
Residual	1	tri-n-butyl citrate	0.7193	N					
	2	ethidium bromide	0.9288	N	trinitrotoluene (TNT)	0.9193	sodium azide	0.9150	7
Residual	2	triaminoguanidinium dinitropyrazolopyrazole	0.7205	N					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
	3	ethidium bromide	0.9271	N	triaminoguanidinium dinitropyrazolopyrazole	0.9129	1,1-bi-2-napthol	0.9123	7
Residual	3	hydroquinine	0.7470	N					
Ammonium Nitrate: Sugar (80:20)	1	sucrose	0.8209	Y	vanilla pudding Jello instant	0.6956	Aspartame_Shop Rite Sugar Sub.	0.6736	2
Residual	1	terephthalic acid	0.7480	N					
	2	sucrose	0.7493	Y	vanilla pudding Jello instant	0.7262	Aspartame_Shop Rite Sugar Sub.	0.6824	3
Residual	2	1,2,4-trichlorobenzene	0.7136	N					
	3	sucrose	0.8447	Y	vanilla pudding Jello instant	0.7706	Aspartame_Shop Rite Sugar Sub.	0.7201	2
Residual	3	terephthalic acid	0.7590	N					
Ammonium Nitrate: Sugar (60:40)	1	sucrose	0.8222	Y	vanilla pudding Jello instant	0.6830	Aspartame_Shop Rite Sugar Sub.	0.6709	2
Residual	1	terephthalic acid	0.7490	N					
	2	thallium(ous) nitrate	0.9752	N	ammonium nitrate	0.9645	Mn (II) nitrate tetrahydrate	0.8993	5
Residual	2	terephthalic acid	0.7860	N					
	3	sucrose	0.8186	Y	vanilla pudding Jello instant	0.7193	Aspartame_Shop Rite Sugar Sub.	0.6935	2
Residual	3	terephthalic acid	0.7560	N					
Ammonium Nitrate: Sugar (50:50)	1	Bis(triaminoguanidinium)-5,5-azotetrazole	0.7455	N	Sucrose	0.7388	methyl-o-nitro benzoate	0.7026	6
Residual	1	sucrose	0.7130	Y					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
	2	ammonium nitrate	0.9854	Y	thallium(ous) nitrate	0.9612	Silver nitrate	0.9332	5
Residual	2	terephthalic acid	0.7890	N					
	3	Astrolite G	0.8299	N	ammonium nitrate	0.8292	samarium (III) nitrate 6H2O	0.8210	7
Residual	3	tetramethylene sulfoxide	0.7480	N					
Ammonium Nitrate: Sugar (40:60)	1	sucrose	0.8421	Y	Aspartame_Shop Rite Sugar Sub.	0.7457	dextrose anhydride	0.7383	2
Residual	1	terephthalic acid	0.7380	N					
	2	vanilla pudding Jello instant	0.9071	N	table sugar	0.9028	sugar_Shoprite confections	0.7765	2
Residual	2	terephthalic acid	0.7490	N					
	3	sucrose	0.7630	Y	1-bromo-2-nitrobenzene	0.6967	3,4-dinitrotoluene	0.6961	3
Residual	3	3,4-dinitrotoluene	0.7160	N					
Ammonium Nitrate: Sugar (30:70)	1	3,4-dinitrotoluene	0.7399	N	2,5-pyridine dicarboxylic acid	0.7226	ethidium bromide	0.7101	7
Residual	1	sucrose	0.7490	Y					
	2	sugar_Shoprite pure cane	0.8487	Y	vanilla pudding Jello instant	0.8162	Nutrasweet	0.8154	7
Residual	2	terephthalic acid	0.7380	N					
	3	sucrose	0.8490	Y	vanilla pudding Jello instant	0.8135	Aspartame_Shop Rite Sugar Sub.	0.7721	1
Residual	3	terephthalic acid	0.7680	N					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Ammonium Nitrate: Cumin (80:20)	1	vinyl chloride 90% vinyl acetate 10%	0.6980	N	pyridoxine HCl	0.6765	2-chloropentafluoro-1,3-butadiene	0.6710	7
Residual	1	vinyl chloride 90% vinyl acetate 10%	0.6980	N					
	2	ammonium nitrate	0.7366	Y	Mn (II) nitrate tetrahydrate	0.7330	silver nitrate	0.7246	6
Residual	2	tetramethylene sulfoxide	0.8380	N					
	3	vinyl chloride 90% vinyl acetate 10%	0.7242	N	tetramethylene sulfoxide	0.6723	lithium tetraborate	0.6544	4
Residual	3	vinyl chloride 90% vinyl acetate 10%	0.7240	N					
Ammonium Nitrate: Cumin (60:40)	1	Mn (II) nitrate tetrahydrate	0.8017	N	lead nitrate	0.8014	silver nitrate	0.7900	7
Residual	1	terephthalic acid	0.7330	N					
	2	silver nitrate	0.9346	N	ammonium nitrate	0.9319	Mn (II) nitrate tetrahydrate	0.9307	7
Residual	2	terephthalic acid	0.7920	N					
	3	methyl-5-methyl-2-furoate	0.6547	N	5-methyl-2-furonitrite	0.6296	Alcian Blue Pyridine Variant	0.5756	7
Residual	3	methyl-5-methyl-2-furoate	0.6540	N					
Ammonium Nitrate: Cumin (50:50)	1	ALL <0.6000							
Residual	1	N/A ALL <0.6000							
	2	lead nitrate	0.8258	N	silver nitrate	0.8058	selenium (ICP calibration)	0.7793	7
Residual	2	terephthalic acid	0.7890	N					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
	3	merquiracine	0.7831	N	2-methylnaphthol [1,2-d] thiazole	0.7661	2-acetyl3-methyl thiophene	0.7655	7
Residual	3	merquiracine	0.7830	N					
Ammonium Nitrate: Cumin (40:60)	1	3-phenyl-6-benzoyl-a-pyrene	0.7391	N	syringaldazine	0.7069	oxalacetic acid diethyl ester	0.6575	7
Residual	1	3-phenyl-6-benzoyl-a-pyrene	0.7450	N					
	2	vinyl chloride 90% vinyl acetate 10%	0.7228	N	dimethyl sulfoxide	0.6686	periodic acid	0.6647	5
Residual	2	vinyl chloride 90% vinyl acetate 10%	0.7230	N					
	3	ALL <0.6000							
Residual	3	N/A ALL <0.6000							
Ammonium Nitrate: Cumin (30:70)	1	tri-n-butyl citrate	0.6204	N	Naphthol Red 22	0.6100	x	x	x
Residual	1	tri-n-butyl citrate	0.6200						
	2	vinyl chloride 90% vinyl acetate 10%	0.6330	N	2-chloropentafluoro-1,3-butadiene	0.6206	tetramethylene sulfoxide	0.6057	6
Residual	2	vinyl chloride 90% vinyl acetate 10%	0.6330	N					
	3	ethidium bromide	0.7840	N	B-naphthol	0.7661	trinitrotoluene (TNT)	0.7552	7
Residual	3	B-naphthol	0.7230	N					
SPECIFICITY									
d,l-amphetamine sulfate	1	amphetamine SO4	0.7327	Y	aspartame	0.7284	hydrobenzoin	0.6915	5
	2	aspartame	0.6814	N	2,9-dimethyl-4,7-diphenyl-1,10-	0.6602	hydrobenzoin	0.6533	7

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
	3	3,5-difluoronitro benzene	0.8042	N	2,9-dimethyl-4,7-diphenyl-1,10-	0.7551	2,3-dinitrotoluene	0.7746	7
MDMA	1	Windex vinegar glass cleaner	0.7317	N	pain "relieving" gel_mineral ice	0.7094	tungstic anhydride	0.7039	3
	2	dimethyl hydrazine	0.7511	N	tungstic anhydride	0.7500	Windex vinegar-glass cleaner	0.7209	6
	3	piperonylamine	0.8357	N	tungstic anhydride	0.7735	silver chromate	0.7720	5
MDA	1	Triaminoguanidinium dinitropyrazolopyrazole	0.6486	N	2-methyl-1-nitro-naphthalene	0.6301	tungstic anhydride	0.6278	6
	2	Triaminoguanidinium dinitropyrazolopyrazole	0.7096	N	2-methyl-1-nitro-naphthalene	0.7035	trinitrotoluene (TNT)	0.6989	7
	3	4-methyl-2-nitrobenzoic acid	0.7337	N	Sesamol	0.7222	4-bromo-3-nitroanisole	0.7103	7
MDEA	1	Triaminoguanidinium dinitropyrazolopyrazole	0.6636	N	2,1,3-benzo thiadiazole	0.6614	tungstic anhydride	0.6518	6
	2	tungstic anhydride	0.7017	N	Windex vinegar-glass cleaner	0.6737	pain "relieving" gel-mineral ice	0.6711	6
	3	piperonylamine	0.7498	N	Sesamol	0.7414	4-bromo-3-nitroanisole	0.7335	7
morphine sulfate	1	B-naphthol	0.7402	N	acridine orange channel	0.7021	E-thiocaprolactam	0.6875	7
	2	vinyl chloride 90% vinyl acetate 10%	0.7375	N	acridine orange channel	0.6837	B-naphthol	0.6710	6
	3	B-naphthol	0.7111	N	vinyl chloride 90% vinyl acetate 10%	0.6978	acridine orange channel	0.6928	7
codeine sulfate	1	vinyl chloride 90% vinyl acetate 10%	0.7064	N	titanium IV oxide 99.9%	0.6969	make-up Sephora All Over Color	0.6920	7
	2	vinyl chloride 90% vinyl acetate 10%	0.7050	N	titanium IV oxide 99.9%	0.6830	make-up Sephora All Over Color	0.6794	6

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
	3	trimethyl (trifluoro methyl) silane	0.7549	N	bis(trimethylsilyl) malonate	0.7541	ethyl thioacetate	0.7356	7
benzocaine	1	ethyl-p-amino benzoate	0.9801	Y	dichloromaleic anhydride	0.9472	ethyl p-hydroxy benzoate	0.9001	3
	2	ethyl-p-amino benzoate	0.9642	Y	dichloromaleic anhydride	0.8890	ethyl p-hydroxy benzoate	0.8736	4
	3	dichloromaleic anhydride	0.9418	N	ethyl-p-amino benzoate	0.9233	4-hydroxy benzoic acid methyl ester	0.8889	4
lidocaine	1	DL-camphoric acid	0.6612	N	ketamine	0.6054	fructose	0.6007	7
	2	DL-camphoric acid	0.6307	N	fructose	0.6235	x	x	x
	3	(1)-1,2-bis ((2S,5S)-2,5d	0.7121	N	diethoxy (methyl) vinyl silane	0.6781	2-chloropropane	0.6660	7
procaine	1	1,4-phenylene diamine	0.7365	N	p-iso-propyl benzaldehyde	0.7328	dichloromaleic anhydride	0.7181	6
	2	p-iso-propyl benzaldehyde	0.7326	N	4-carboxy benzaldehyde	0.7186	p-hydroxy benzoic acid	0.7111	4
	3	dichloromaleic anhydride	0.8117	N	ethyl-p-amino benzoate	0.8041	ethyl-4-(butylamino	0.7556	6
acetylsalicylic acid (ASA)	1	acetylsalicylic acid	0.8929	Y	4,4'-biphenyl dicarboxylic acid	0.6875	o-fluorobenzoic acid	0.6822	3
Residual	1	tetramethylene sulfoxide	0.7350	N					
	2	acetylsalicylic acid	0.9224	Y	N,N'-bis(3-methyl phenyl)-N,N'-	0.8074	2-bromofluorene	0.7857	3
Residual	2	tetramethylene sulfoxide	0.7470	N					
	3	acetylsalicylic acid	0.8908	Y	N,N'-bis(3-methyl phenyl)-N,N'-	0.7956	2-bromofluorene	0.7701	3
Residual	3	tetramethylene sulfoxide	0.7407	N					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
ibuprofen	1	hydroxybutyric acid	0.8694	N	ibuprofen_CVS junior strength	0.8077	4,4'-isopropyl idene diphenol	0.7773	6
	2								
	3	hydroxybutyric acid	0.8294	N	6-(trifluoro methyl) pyridine-3-meOH	0.7982	4-sec-butylphenol	0.7866	7
guaifenesin	1	guaiacol glycyryl ether	0.8630	Y	4-bromo veratrole	0.6975	iso-amyl alcohol	0.6668	5
	2	guaiacol glycyryl ether	0.8570	Y	4-bromo veratrole	0.7006	2-methoxy-N-methylaniline	0.6755	6
	3	guaiacol glycyryl ether	0.8831	Y	4-bromo veratrole	0.7072	2-methoxy-N-methylaniline	0.6770	6
diphenhydramine	1	ethyl phenylacetate	0.9231	N	methyl phenylacetate	0.9180	dibenzylamine	0.9136	7
	2	ethyl phenylacetate	0.9113	N	acetaldehyde phen ethyl propyl acetal	0.9011	methyl phenyl acetate	0.8990	6
	3	ethyl phenylacetate	0.9295	N	diazepam	0.9208	butyl phenylacetate	0.9168	6
chlorpheniramine	1	chlorphenir amine maleate	0.7281	Y	B-naphthol	0.6971	2,9-dimethyl-4,7-diphenyl-1,10-	0.6970	7
	2	3,4-dinitrotoluene	0.7208	N	2,3-dinitrotoluene	0.7175	ethidium bromide	0.7098	7
	3	dipyridamole	0.7127	N	chlorphenir amine maleate	0.7005	B-naphthol	0.6923	7
pseudoephedrine	1	Promethazine	0.9521	N	benzyl acetate	0.8729	methyl phenyl acetate	0.8686	7
	2	dibenzyl N,N-diiso propyl phoramidite	0.9116	N	N,1-benzyl-3-pyrrolidinol	0.8995	promethazine	0.8980	7
	3	promethazine	0.8969	N	dibenzyl N,N-diiso propyl phoramidite	0.8868	1-benzyl-3-pyrrolidinol	0.8775	7
Dimethyl sulfone (DMS)	1	methyl sulfone	0.9449	Y	dichloromethane	0.8668	vanadium pentoxide	0.7318	3

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
	2	methyl sulfone	0.9368	Y	dichloromethane	0.8364	2,3-difluorophenol	0.7838	1
	3	dimethyl sulfone	0.8985	Y	dichloromethane	0.7962	dichloro methane	0.7962	1
Baking soda	1	ammonium nitrate	0.9070	N	silver nitrate	0.8960	Mn (II) nitrate tetrahydrate	0.8937	6
	2	silver nitrate	0.8991	N	lead nitrate	0.8956	Mn (II) nitrate tetrahydrate	0.8939	5
	3	bicarb standard	0.9389	Y	silver nitrate	0.9105	lead nitrate	0.9101	5
Acetaminophen (ACE)	1	4-acetamido phenol	0.9071	Y	p-aceto phenetidide	0.8067	4-amino-3-hydrazino-5-mercapto-1,2,4	0.6651	1
Residual	1	tetramethylene sulfoxide	0.7360	N					
	2	Tylenol	0.8848	Y	p-aceto phenetidide	0.7765	4'-amino acetanilide	0.7487	1
Residual	2	tetramethylene sulfoxide	0.7550	N					
	3	Tylenol	0.8814	Y	phenacetin	0.7707	4'-amino acetanilide	0.7060	1
Residual	3	tetramethylene sulfoxide	0.7490	N					
urea	1	guanidine	0.9372	N	lithium sulfate	0.9314	calcium sulfide dihydrate	0.9153	5
	2	lithium sulfate	0.9404	N	calcium sulfate hemihydrate	0.9392	calcium sulfide dihydrate	0.9375	5
	3	1,3,5-trifluoro benzene	0.8761	N	3-fluoro-5-trifluoro methyl benzylamine	0.8691	guanidine	0.8436	6
ferric nitrate	1	barium nitrate	0.9517	N	lanthanum nitrate	0.9486	chromium nitrate	0.9475	6
	2	barium oxide	0.8579	N	calcium pyrophosphate	0.8392	cesium nitrate	0.7968	7

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
	3	chromium nitrate	0.9371	N	aluminum nitrate	0.9227	potassium nitrate	0.9188	7
sodium perborate	1	bleach_chlorox; sodium hydrophosphite 6%	0.6180	N	concrete etcher and rust remover_Behr no	0.6092	choline chloride	0.6090	7
	2	3-chloro-2-fluoro 5-(trifluoromethyl) pyridine	0.7170	N	sodium perborate	0.7091	1,2-epoxy-2-methyl propane	0.6846	7
	3	1,2-epoxy-2-methyl propane	0.6920	N	sodium perborate monohydrate	0.6900	3-chloro-2-fluoro 5-(trifluoromethyl) pyridine	0.6887	6
fertilizer (13% total N) prills	1	aluminum sulfide	0.9573	N	sulfur	0.9259	lead thiosulfate	0.9177	3
Residual	1	aluminum sulfide	0.7590	N					
	2	sulfur	0.9788	N	aluminum sulfide	0.9250	potash, sulfurated	0.9124	3
Residual	2	terephthalic acid	0.7820	N					
	3	sulfur	0.9713	N	potash, sulfurated	0.9241	aluminum sulfide	0.8842	3
Residual	3	terephthalic acid	0.7850	N					
fertilizer (13% total N) ground	1	lead styphnate	0.9147	N	2,4-dinitrophenyl hydrazine	0.8528	N,N-ethyl-N-(2-nitroxyethyl) nitramine	0.7967	7
Residual	1	lead styphnate	0.8200	N					
	2	lead styphnate	0.8698	N	2,4-dinitrophenyl hydrazine	0.8188	lanthanum iodide	0.8117	6
Residual	2	lanthanum iodide	0.7640	N					
	3	lead styphnate	0.6796	N	sulfur	0.6417	2,4-dinitrophenyl hydrazine	0.6401	5

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Residual	3	Rhodium (III) acetylacetonate	0.6860	N					
Turmeric : cardamom (50:50)	1	ammonium chloride	0.6507	N	x	x	x	x	x
Residual	1	ammonium chloride	0.6550	N					
	2	vinyl chloride 90% vinyl acetate 10%	0.7336	N	tetramethylene sulfoxide	0.6819	lithium tetraborate	0.6770	5
Residual	2	tetramethylene sulfoxide	0.7748	N					
	3	trans-2-dodecenal	0.5966	N	2-methyl-2 pentenal	0.5861	4-chlorocinnamic acid	0.5515	7
Residual	3	trans-2-dodecenal	0.5970	N					
sodium hydroxide (lye)	1	ethidium bromide	0.8115	N	trinitrotoluene (TNT)	0.7944	Sodium formate	0.7897	7
	2	ethidium bromide	0.8638	N	trinitrotoluene (TNT)	0.8362	Triaminoguanidinium dinitropyrazolopyrazole	0.8343	7
	3	ethidium bromide	0.8216	N	2-nitrofuran	0.7989	3,4-dinitrotoluene	0.7987	7
sulfuric acid	1	sulfuric acid (conc.)	0.9603	Y	phosphoric Acid	0.8181	hydrophosphorus acid	0.8158	4
	2	sulfuric acid	0.9609	Y	phosphoric Acid	0.8622	hydrophosphorus acid	0.8286	6
	3	sulfuric acid(conc)	0.9757	Y	phosphoric Acid	0.8602	hydrophosphorus acid	0.8413	3
ammonium hydroxide	1	sodium formate	0.7768	N	ethidium bromide	0.7538	2,3-dinitrotoluene	0.7442	7
	2	ethidium bromide	0.7777	N	Sodium Formate	0.7776	2,3-dinitrotoluene	0.7734	7
	3	ethidium bromide	0.7959	N	2,3-dinitrotoluene	0.7820	3,4 DNT	0.7771	7

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
citric acid	1	citric acid anhydride	0.8046	Y	dimethyl 2,3-o-iso propylidene-L-tartrate	0.6864	sodium phosphate	0.6684	2
	2	citric acid	0.8144	Y	L-aspartic acid	0.7085	dimethyl 2,3-o-iso propylidene-L-tartrate	0.6681	2
	3	citric acid	0.7448	Y	ethyl nitroacetate	0.6942	L-aspartic acid	0.6918	3
RUGGEDNESS									
cocaine HCl	1	Icocaine2	0.8238	Y	ibuprofen	0.8213	Ethylene glycol phenyl ether methacrylate	0.8051	7
	3	Icocaine2	0.8778	Y	ibuprofen	0.8736	Ethylene glycol phenyl ether methacrylate	0.8462	5
methamphetamine	1	mescaline	0.7886	N	Valium tab 1	0.7721	z-L-isoluecine	0.7713	6
	3	cis-1,3-o-benzylidene glycerol	0.8175	N	o-benzyl-L-serine	0.7989	2,3,4,6-tetra-o-benzyl-alpha-D-glucopyranosyl	0.7936	7
caffeine	1	caffeine	0.8311	Y	potassium stannate trihydrate	0.7872	tetramethyl thiuram	0.7620	6
	3	caffeine	0.8929	Y	butalbital	0.7764	tetramethyl thiuram disulfide	0.7754	5
ammonium nitrate (powder)	1	ammonium nitrate	0.9902	Y	zirconium (IV) sulfate hydrate	0.9449	thallium(ous) nitrate	0.9414	6
	3	thallium(ous) nitrate	0.9849	N	ammonium nitrate	0.9591	bismuth (III) subnitrate monohydrate	0.9440	5
ammonium perchlorate	1	silver perchlorate monohydrate	0.9152	N	silver perchlorate	0.9129	zinc perchlorate hexahydrate	0.9011	6
	3	zinc perchlorate 6H2O	0.9784	N	cesium perchlorate	0.9668	manganese (II) perchlorate 6H2O	0.9659	6
RDX	1	RDX Type2 Class 3	0.7138	Y	2-nitroethanol	0.7113	acetamide	0.6892	5
	3	RDX	0.8151	Y	hydrogen peroxide 30%	0.7866	RDX Type2 Class 3	0.7693	3

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
BP® 87 Octane Gasoline	1	contact adhesive	0.8417	N	Weld Wood contact cement-dap	0.8288	3-(3-Methoxy phenyl)propionic acid	0.8229	6
Residual	1	tetramethylene sulfoxide	0.7330	N					
	3	3-benzylaniline	0.9259	N	lacquer thinner_Klean Strip	0.9031	contact adhesive	0.9011	7
Residual	3	lacquer thinner	0.6110	N					
BP® diesel fuel	1	fuel injection cleaner Pennzoil Gumout	0.9017	N	1-dodecanethiol	0.8968	cholesteryl myristate	0.8948	6
Residual	1	tributyl citrate	0.8020	N					
	3	paint thinner	0.9360	N	adhesive remover and cleaning solvent	0.9317	Prestone 0 to 60 Booster	0.9302	7
Residual	3	zinc oxalate hydrate	0.4030	N					
PORTABILITY									
PREVIOUS ID:									
9: NCSD, Fake cocaine base	1	Tylenol	0.7608	Y	phenacetin	0.7072	4-Nitro-3-(trifluoro methyl) phenol	0.7021	2
Residual	1	tetramethylene sulfoxide	0.7590	N					
9	2	4-Nitro-3-(trifluoro methyl)phenol	0.8286	N	3,5-dinitro salicylic acid	0.8043	8-anilino-1-naphth alene-sulfonic acid	0.7838	6
Residual	2	4-Nitro-3-(trifluoro methyl)phenol	0.8120	N					
9	3	4-Nitro-3-(trifluoro methyl)phenol	0.8174	N	3,5-dinitro salicylic acid	0.7969	8-anilino-1-naphth alene-sulfonic acid	0.7786	6
Residual	3	4-Nitro-3-(trifluoro methyl)phenol	0.8010	N					
10: Cocaine base	1	(Carbethoxyethylid ene)triphenyl phosphorane	0.8076	N	Benzyl phenyl sulfide	0.8052	Tetraphenylphos phonium chloride	0.8037	7

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Residual	1	3-methyl-1-phenyl-2-pyrazolin-5-one	0.7139	N					
10	2	QuadraPure™ AEA	0.7518	N	R-3,3'-Bis(triphenyl silyl)-1,1'-bi-2-naphthol	0.7510	N,N-Diphenyl formamide	0.7509	7
Residual	2	tetramethylene sulfoxide	0.7290	N					
10	3	3,5-Difluoro nitrobenzene	0.8197	N	R-3,3'-Bis(triphenyl silyl)-1,1'-bi-2-naphthol	0.7380	8-anilino-1-naphth alene-sulfonic acid	0.7202	7
Residual	3	3,5-Difluoro nitrobenzene	0.7950	N					
34: HEROIN	1	vinyl chlorate 90% vinyl acetate 10%	0.7508	N	2-acetylcyclo hexanone	0.6943	tetramethylene sulfoxide	0.6817	7
Residual	1	tetramethylene sulfoxide	0.7830	N					
34	2	All <0.60							
Residual	2	All <0.60							
34	3	vinyl chlorate 90% vinyl acetate 10%	0.7356	N	lithium tetraborate	0.6880	tetramethylene sulfoxide	0.6786	7
Residual	3	vinyl chlorate 90% vinyl acetate 10%	0.7360	N					
35: Heroin	1	vinyl chlorate 90% vinyl acetate 10%	0.7455	N	2-acetylcyclo hexanone	0.6944	pyroxidine HCl	0.6913	7
Residual	1	tetramethylene sulfoxide	0.7895	N					
35	2	All <0.60							
Residual	2	All <0.60							

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
35	3	vinyl chlorate 90% vinyl acetate 10%	0.7579	N	Periodic Acid	0.7211	ethyl-2-,3 dibromo propionate	0.7107	4
Residual	3	vinyl chlorate 90% vinyl acetate 10%	0.7579	N					
38: Heroin	1	vinyl chlorate 90% vinyl acetate 10%	0.8080	N	tetramethylene sulfoxide	0.7193	periodic acid	0.7159	4
Residual	1	tetramethylene sulfoxide	0.8419	N					
38	2	vinyl chlorate 90% vinyl acetate 10%	0.8099	N	periodic acid	0.7443	ethyl-2,3 dibromo propionate	0.7280	4
Residual	2	vinyl chlorate 90% vinyl acetate 10%	0.8087	N					
38	3	vinyl chlorate 90% vinyl acetate 10%	0.7371	N	tetramethylene sulfoxide	0.6954	ethyl-2,3 dibromo propionate	0.6628	4
Residual	3	tetramethylene sulfoxide	0.8300	N					
39: Heroin	1	3-phenyl-6-benzoyl-a-pyrone	0.7269	N	syringaldazine	0.6881	gadolinium (III) oxide	0.6693	7
Residual	1	3-phenyl-6-benzoyl-a-pyrone	0.7783	N					
39	2	gadolinium (III) oxide	0.6612	N	1,5-Bis(4-aminophenyl) penta-1,4-diene-3-	0.6511	Methyl 2-oxo-2H-pyran-3-carboxylate	0.6413	7
Residual	2	gadolinium (III) oxide	0.6672	N					
39	3	Poly(acrylic acid-co-maleic acid) sol'n	0.7482	N	Poly(acrylic acid) partial Na salt sol'n	0.7278	4,5-dimethyl-3-hydroxy-2,5-dihydro furan-2-	0.6740	7
Residual	3	Poly(acrylic acid-co-maleic acid) sol'n	0.7582	N					
44B: Cocaine base	1	QuadraPure™ IMDAZ	0.7320	N	QuadraPure™ AEA	0.7237	Ethyl 3-methyl-3-phenylglycidate	0.7180	7
Residual	1	tetramethylene sulfoxide	0.7347	N					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
44B	2	QuadraPure™ AEA	0.7578	N	QuadraPure™ IMDAZ	0.7465	Ethyl 3-methyl-3-phenylglycidate	0.7458	7
Residual	2	tetramethylene sulfoxide	0.7664	N					
44B	3	3,5-Difluoro nitrobenzene	0.8082	N	triaminoguanidinium dinitropyrazolopyrazole	0.7435	3,4-dinitrotoluene	0.7362	7
Residual	3	tri-n-butyl citrate	0.7121	N					
49B: Cocaine base	1	QuadraPure™ IMDAZ	0.7688	N	QuadraPure™ AEA	0.7677	Ethyl 3-methyl-3-phenylglycidate	0.7544	7
Residual	1	tetramethylene sulfoxide	0.7504	N					
49B	2	3,5-Difluoro nitrobenzene	0.7977	N	1-phenyl-1H-tetrazole-5-thiol	0.7265	5-nitroisophtahlic acid	0.7083	7
Residual	2	1-phenyl-1H-tetrazole-5-thiol	0.7077	N					
49B	3	3,5-Difluoro nitrobenzene	0.8329	N	5-nitroisophtahlic acid	0.7468	3,4-dinitrotoluene	0.7404	7
Residual	3	3,5-Difluoro nitrobenzene	0.7716	N					
50: Cocaine HCl	1	3,5-Difluoro nitrobenzene	0.8297	N	R-3,3'-Bis(triphenyl silyl)-1,1'-bi-2-naphthol	0.7494	1-Fluoro-3-iodo-5-nitrobenzene	0.7376	7
Residual	1	3,5-Difluoro nitrobenzene	0.8036	N					
50	2	R-3,3'-Bis(triphenyl silyl)-1,1'-bi-2-naphthol	0.7747	N	4,4'-Methylene diantipyrine	0.7494	3-methyl-1-phenyl-2-pyrazolin-5-one	0.7454	7
Residual	2	tetramethylene sulfoxide	0.7160	N					
50	3	Icocaine2	0.7935	Y	3-methyl-1-phenyl-2-pyrazolin-5-one	0.7885	ibuprofen	0.7862	7

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Residual	3	tetramethylene sulfoxide	0.7590	N					
501: 7.5mg Hydrocodone/ 500mg ACE (LORTAB)	1	Tylenol	0.8651	Y	phenacetin	0.7730	4'-amino acetanilide	0.7270	1
Residual	1	tetramethylene sulfoxide	0.7521	N					
501	2	Tylenol	0.8637	Y	phenacetin	0.7549	4'-amino acetanilide	0.7077	1
Residual	2	tetramethylene sulfoxide	0.7527	N					
501	3	Tylenol	0.7844	Y	phenacetin	0.7074	4-Nitro-3-(trifluoro methyl) phenol	0.6814	2
Residual	3	tetramethylene sulfoxide	0.7523	N					
502: 100mg Propoxyphene/ 650 ACE (DARVOCET)	1	Tylenol	0.8208	Y	phenacetin	0.7439	4'-aminoacetanilide	0.7061	1
Residual	1	tetramethylene sulfoxide	0.7547	N					
502	2	Tylenol	0.7903	Y	phenacetin	0.7264	2,5-dinitrophenol	0.6848	1
Residual	2	tetramethylene sulfoxide	0.7523	N					
502	3	Tylenol	0.8349	Y	phenacetin	N	4'-amino acetanilide	0.6988	1
Residual	3	tetramethylene sulfoxide	0.7550	N					
503: 15mg Oxycodone HCl (ROXICODONE)	1	4-Nitro-3-(trifluoro methyl)phenol	0.8383	N	3,4-dinitrotoluene	0.8144	4,6-dinitro-o-cresol	0.7648	7
Residual	1	3,4-dinitrotoluene	0.7745	N					
503	2	4-Nitro-3-(trifluoro methyl)phenol	0.8499	N	3,4-dinitrotoluene	0.8224	3,5-dinitro salicylic acid	0.8107	7

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Residual	2	3,4-dinitrotoluene	0.7963	N					
503	3	vinyl chlorate 90% vinyl acetate 10%	0.6767	N	E-thiocaprolactam	0.6763	eye shadow_ Loreal lily	0.6449	7
	3	tetramethylene sulfoxide	0.7045	N					
504: 30mg Oxycodone HCl (ROXICODONE)	1	4-Nitro-3-(trifluoro methyl)phenol	0.7433	N	3,4-dinitrotoluene	0.7343	chloramphenicol	0.7140	7
Residual	1	3,4-dinitrotoluene	0.6682	N					
504	2	4-Nitro-3-(trifluoro methyl)phenol	0.6858	N	3,4-dinitrotoluene	0.6853	2,4-dinitrotoluene	0.6687	7
Residual	2	vinyl chlorate 90% vinyl acetate 10%	0.6812	N					
504	3	B-naphthol	0.7376	N	3,4-dinitrotoluene	0.7300	4-Nitro-3-(trifluoro methyl) phenol	0.7227	7
Residual	3	B-naphthol	0.7376	N					
505: Cocaine base	1	QuadraPure™ AEA	0.7954	N	Ethyl 3-methyl-3-phenylglycidate	0.7901	Aniline, polymer bound	0.7803	7
Residual	1	tetramethylene sulfoxide	0.7857	N					
505	2	QuadraPure™ AEA	0.7950	N	QuadraPure™ IMDAZ	0.7864	Aniline, polymer bound	0.7747	7
Residual	2	tetramethylene sulfoxide	0.7507	N					
505	3	QuadraPure™ AEA	0.7319	N	p-dibenzyloxi benzene	0.7244	1-phenyl-1H-tetrazole-5-thiol	0.7241	7
Residual	3	tri-n-butyl citrate	0.7585	N					
506: 2 mg Alprazolam (Xanax)	1	a-lactose	0.8222	N	4-Nitro-3-(trifluoro methyl)phenol	0.7981	3,4-dinitrotoluene	0.7711	7

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Residual	1	3,4-dinitrotoluene	0.7840	N					
506	2	4-Nitro-3-(trifluoro methyl)phenol	0.8461	N	3,5-dinitrosalicylic acid	0.8089	B-naphthol	0.7982	7
Residual	2	B-naphthol	0.8050	N					
506	3	4-Nitro-3-(trifluoro methyl)phenol	0.8344	N	3,5-dinitrosalicylic acid	0.7954	1-bromo-4-nitro benzene	0.7948	7
Residual	3	4-Nitro-3-(trifluoro methyl)phenol	0.8210	N					
507: Cocaine base	1	3,5-difluoro nitrobenzene	0.8721	N	Triaminoguanidinium dinitropyrazolopyrazole	0.8351	3,4-dinitrotoluene	0.8223	7
Residual	1	3,4-dinitrotoluene	0.7497	N					
507	2	3,4-dinitrotoluene	0.8582	N	3,5-difluoro nitrobenzene	0.8428	ethidium bromide	0.8385	7
Residual	2	3,4-dinitrotoluene	0.8582	N					
507	3	3,5-difluoro nitrobenzene	0.8501	N	ethidium bromide	0.8244	Triaminoguanidinium dinitropyrazolopyrazole	0.8213	7
Residual	3	3,4-dinitrotoluene	0.7669	N					
508: Lidocaine	1	ketamine	0.6854	N	6-methylquinoline	0.6274	Sodium tartrate dibasic dihydrate	0.6160	7
Residual	1	terephthalic acid	0.7340	N					
508	2	ketamine	0.8049	N	<0.60		<0.60		
Residual	2	terephthalic acid	0.7470	N					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
508	3	ketamine	0.6412	N	<0.60				
Residual	3	terephthalic acid	0.7310	N					
509: 10mg Methadone HCl (METHADONE)	1	4-Nitro-3-(trifluoro methyl) phenol	0.8577	N	3,4-dinitrotoluene	0.8214	3,5-dinitro salicylic acid	0.8104	7
Residual	1	3,4-dinitrotoluene	0.7907	N					
509	2	4-Nitro-3-(trifluoro methyl) phenol	0.8406	N	3,4-dinitrotoluene	0.8123	a-lactose	0.7975	7
Residual	2	starch	0.7986	N					
509	3	4-Nitro-3-(trifluoro methyl) phenol	0.8663	N	3,5-dinitro salicylic acid	0.8239	3,4-dinitrotoluene	0.8205	7
Residual	3	3,4-dinitrotoluene	0.7875	N					
510: Cocaine base	1	QuadraPure™ AEA	0.8347	N	phenylboronic acid pinacol ester	0.8232	Aniline, polymer bound	0.8222	7
Residual	1	tetramethylene sulfoxide	0.7855	N					
510	2	QuadraPure™ AEA	0.7634	N	3,5-difluoronitro benzene	0.7542	QuadraPure™ IMDAZ	0.7456	7
Residual	2	tri-n-butyl citrate	0.7726	N					
510	3	QuadraPure™ AEA	0.8643	N	Aniline, polymer bound	0.8566	QuadraPure™ IMDAZ	0.8529	7
Residual	3	tetramethylene sulfoxide	0.7754	N					
511: Heroin	1	acridine orange channel	0.7299	N	2,3,4-trifluoro nitrobenzene	0.7143	Ethidium Bromide	0.7091	7
Residual	1	acridine orange channel	0.7298	N					
511	2	pyridoxine HCl	0.7050	N	acridine, orange channel	0.7020	vinyl chlorate 90% vinyl acetate 10%	0.7009	7

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Residual	2	pyridoxine HCl	0.7042	N					
511	3	vinyl chlorate 90% vinyl acetate 10%	0.7444	N	2-acetylcyclo hexanone	0.6890	tetramethylene sulfoxide	0.6796	7
Residual	3	vinyl chlorate 90% vinyl acetate 10%	0.7428	N					

Table 2

Point-and-Shoot Sampling Mode

Results are reported as displayed on the instrument.

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
CONFORMITY									
Cocaine HCl	1	ibuprofen	0.7522	N	Icocaine2	0.7472	clorazepate	0.6976	7
	2	ibuprofen	0.6738	N	Icocaine2	0.6675	aspartame	0.6506	7
Cocaine base	1	3,5-difluoronitro benzene	0.8048	N	acridine orange channel	0.7400	ethidium bromide	0.7348	7
Residual	1	acridine orange channel	0.6920	N					
	2	pyridoxine HCl	0.6886	N	lithium tetraborate	0.6759	Basic Blue 6 (Meldola's blue)	0.6670	6
Residual	2	tetramethylene sulfoxide	0.6920	N					
Methamphetamine	1	Valium tab 1	0.6954	N	aspartame	0.6742	mescaline	0.6513	7
	2	aspartame	0.6921	N	Valium tab 1	0.6630	sodium tartrate dibasic dihydrate	0.6609	7
Heroin	1	3,4-dinitrotoluene	0.6811	N	2,3-dinitrotoluene	0.6766	1,2-dimethyl-3-nitrobenzene	0.6181	6
	2	B-naphthol	0.7351	N	3,4-dinitrotoluene	0.7333	triaminoguanidinium dinitropyrazolo-pyrazole	0.7216	7
Mannitol	1	D-sorbitol	0.7733	N	nitroethane	0.7707	sodium D-gluconate	0.7485	4
	2	nitroethane	0.7880	N	D-sorbitol	0.7539	sodium D-gluconate	0.7417	4
Niacinamide	1	niacinamide	0.9432	Y	morphine	0.9197	K hydrogen phthalate	0.8025	3

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
	2	K hydrogen phthalate	0.7379	N	water pump lubricant	0.7374	bis(triaminoguanidinium)-5,5-azotetrazole	0.7314	3
Boric Acid	1	N-methyl acetamide	0.7419	N	nitroethane	0.7319	2-bromo-fluoroaniline	0.7296	5
	2	nitroethane	0.7186	N	ethidium bromide	0.6954	Triaminoguanidinium dinitropyrazolo-pyrazole	0.6783	6
Inositol	1	potassium sodium tartrate	0.7450	N	potassium sodium tartrate	0.7006	3,4-dinitrotoluene	0.6761	7
Caffeine	1	caffeine	0.8855	Y	butalbital	0.8407	sodium bismuthate	0.6276	2
	2	caffeine	0.8536	Y	butalbital	0.7625	hexafluoro benzene	0.6358	3
Quinine	1	hydroquinidine HCl	0.8752	N	1,1-bi-2-naphthol	0.8693	N,N-dimethyl-1-napthylamine	0.8609	7
RDX	1	RDX	0.8188	Y	nitropropane	0.6371	boric acid	0.6323	6
Residual	1	terephthalic acid	0.7470	N					
	2	RDX	0.7617	Y	boric acid	0.6884	nitroethane	0.6862	5
Residual	2	tetramethylene sulfoxide	0.7340	N					
Ammonium Nitrate (prills)	1	ammonium nitrate	0.9336	Y	samarium (III) nitrate 6H2O	0.9156	thallium(ous) nitrate	0.9069	6
Ammonium Nitrate (powder)	1	ammonium nitrate	0.9097	Y	samarium (III) nitrate 6H2O	0.8972	thallium(ous) nitrate	0.8847	6
	2	ammonium nitrate	0.9453	Y	thallium(ous) nitrate	0.9348	samarium (III) nitrate 6H2O	0.9118	6
Ammonium Perchlorate	1	ammonium perchlorate	0.9496	Y	Cobalt (II) perchlorate 6H2O	0.9484	magnesium perchlorate	0.9482	6

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Sugar	1	silver lactate	0.6585	N	3,4-dinitrotoluene	0.6444	sodium tartrate dibasic dihydrate	0.6443	7
Cumin	1	Basic Blue 6 (Meldolas's blue)	0.8398	N	1,2-benzisothiazol-3(2H)-one	0.7663	6-Nitroquinoline	0.7530	7
Residual	1	Basic Blue 6 (Meldolas's blue)	0.8020	N					
Urea Nitrate	1	barium carbonate	0.8090	N	nickel(ous) nitrate	0.8072	Sr Nitrate anhydrous	0.8018	5
	2	barium oxide	0.7606	N	zinc nitrate hydrate	0.7333	Cesium hydrogen carbonate	0.7258	6
Mineral Spirits	1	Imidazole-2-carboxaldehyde	0.8813	N	N,N"-2,4-Hexadiyal-1,6-diylbis (N'-ethyl urea)	0.8600	2-ethyoxy thiazole	0.8565	7
Residual	1	2-ethoxythiazole	0.8430	N					
	2	mineral oil	0.9639	N	Old English lemon oil	0.9635	Nujol	0.9569	6
Residual	2	terephthalic acid	0.7640	N					
BP® 87 Octane Gasoline	1	1-benzyl-2-methylimidiazole	0.8449	N	trans-2-phenylcyclo propyl isocyanate	0.7921	3-benzylaniline	0.7893	7
Residual	1	terephthalic acid	0.7290	N					
	2	contact adhesive	0.8958	N	lacquer thinner	0.8699	Weld Wood Contact Cement	0.8562	5
Residual	2	terephthalic acid	0.7750	N					
BP® Diesel Fuel	1	calcium oxalate monohydrate	0.8505	N	imidazole-2-carboxaldehyde	0.8492	cerium (III) oxalate hydrate	0.8383	7
Residual	1	diethanolamine	0.7940	N					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
	2	mineral oil	0.9503	N	Old English lemon oil	0.9484	fuel inj. cleaner Pennzoil Gumout	0.9419	5
Residual	2	terephthalic acid	0.7830	N					
Kerosene	1	imidazole-2-carboxaldehyde	0.8741	N	calcium oxalate monohydrate	0.8696	N,N"-2,4-hexa diyne-1,6-diylbis(N'-ethyl urea)	0.8648	7
Residual	1	calcium oxalate monohydrate	0.8470	N					
	2	Nujol	0.9741	N	mineral oil	0.9734	Old English lemon oil	0.9713	6
Residual	2	terephthalic acid	0.7890	N					
Klean-Strip® VM&P Naphtha Thinner	1	imidazole-2-carboxaldehyde	0.8828	N	2-ethoxythiazole	0.8723	N,N"-2,4-hexa diyne-1,6-diylbis(N'-ethyl urea)	0.8406	7
Residual	1	2-ethoxythiazole	0.8410	N					
	2	Naphtha VM&P Klean Strip	0.9484	Y	Nujol	0.9395	cetyltrimethyl ammonium chloride	0.9240	5
Residual	2	terephthalic acid	0.7800	N					
Lamplight® lamp oil	1	imidazole-2-carboxaldehyde	0.8759		N,N"-2,4-hexa diyne-1,6-diylbis(N'-ethyl urea)	0.8527	calcium oxalate monohydrate	0.8479	7
Residual	1	2-ethoxythiazole	0.8330	N					
	2	Nujol	0.9725	N	mineral oil	0.9615	Old English lemon oil	0.9575	6
Residual	2	terephthalic acid	0.7810	N					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Ronsonol lighter fuel®	1	imidazole-2-carboxaldehyde	0.8788	N	2-ethoxythiazole	0.8730	N,N''-2,4-hexadiyne-1,6-diylbis(N'-ethyl urea)	0.8475	7
Residual	1	2-ethoxythiazole	0.8390	N					
	2	polyethylenimine solution	0.9337	N	europium	0.9219	kerosene	0.9212	7
Residual	2	tri-n-butyl citrate	0.7710	N					
Kingsford® charcoal lighter fluid	1	imidazole-2-carboxaldehyde	0.8726	N	2-ethoxythiazole	0.8536	N,N''-2,4-hexadiyne-1,6-diylbis(N'-ethyl urea)	0.8493	7
Residual	1	2-ethoxythiazole	0.8270	N					
	2	polyethylenimine solution	0.9465	N	europium	0.9412	kerosene	0.9328	7
Residual	2	tri-n-butyl citrate	0.7810	N					
MIXTURE SENSITIVITY									
Cocaine HCl: Caffeine (80:20)	1	ethylene glycol	0.6683	N	poly(ethylene glycol) phenyl ether acrylate	0.6564	anti-diphenyl glyoxime	0.6517	7
Residual	1	terephthalic acid	0.7650	N					
	2	p-dibenzyl oxibenzene	0.6982	N	tert-butyl (2S,3R)- (-)-6-oxo-2,3,diphenyl-4-	0.6907	(S)-(+)-alpha-methoxyphenyl-acetic acid	0.6806	7
Residual	2	tert-butyl (2S,3R)-(-)-6-oxo-2,3,diphenyl-4-	0.6510	N					
Cocaine HCl: Caffeine (60:40)	1	hydrobenzoin	0.7473	N	R-3,3'-bis(triphenyl silyl)-1-1'-bi-2-naphthol	0.7294	3-aminobenzoic acid	0.7208	6

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Residual	1	tri-n-butyl citrate	0.7170	N					
Cocaine HCl: Caffeine (50:50)	1	hydralazine	0.6374	N	B-naphthol	0.6239	2-methyl naphthol [1,2-a] thiazole	0.6223	7
Residual	1	2,3-dintrotoluene	0.6110	N					
	2	3,5-Difluoronitro benzene	0.7686	N	R-3,3'-bis(triphenyl silyl)-1-1'-bi-naphthol	0.7311	1-phenyl-1H-tetrazole-5-thiol	0.7201	7
Residual	2	1-phenyl-1H-tetrazole-5-thiol	0.7170	N					
Cocaine HCl: Caffeine (40:60)	1	2-methylnaphtho [1,2-d]thiazole	0.6752	N	2-methyl-1-nitro-naphthalene	0.6736	B-naphthol	0.6678	7
Residual	1	2-methylnaphtho [1,2-d]thiazole	0.6750	N					
Cocaine HCl: Caffeine (30:70)	1	tetramethyl thiuram disulfide	0.7047	N	caffeine	0.6478	(bromomethyl) trimethyl silane	0.6217	6
Residual	1	2,3-dinitrotoluene	0.6880	N					
Cocaine base: caffeine (80:20)	1	3,5-difluoronitro benzene	0.8403	N	ethidium bromide	0.8239	triaminoguanidinium dinitropyrazolopyrazole	0.8230	7
Residual	1	3,4-dinitrotoluene	0.7790	N					
Cocaine base: caffeine (60:40)	1	3,5-difluoronitro benzene	0.6419	N	B-naphthol	0.6225	1-(2-bromoethyl) naphthalene	0.6019	0
Residual	1	tetramethylene sulfoxide	0.6970	N					
Cocaine base: caffeine (50:50)	1	tetramethyl thiuram disulfide	0.6676	N	caffeine	0.6372	2,3-dinitrotoluene	0.6201	6
Residual	1	2,3-dinitrotoluene	0.7150	N					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
	2	caffeine	0.7228	Y	B-naphthol	0.7113	4-nitro-3-(trifluoro methyl)phenol	0.7040	6
Residual	2	3,4-dinitrotoluene	0.7620	N					
Cocaine base: caffeine (40:60)	1	tetramethyl thiuram disulfide	0.6609	N	B-naphthol	0.6522	2-bromo-3-methyl-thiophene	0.6471	6
Residual	1	tetramethylene sulfoxide	0.6980	N					
Cocaine base: caffeine (30:70)	1	tetramethyl thiuram disulfide	0.7121	N	caffeine	0.6870	(bromomethyl) trimethyl silane	0.6675	6
Residual	1	2,3-dinitrotoluene	0.6910	N					
Methamphetamine: DMS (80:20)	1	hydrobenzoin	0.7280	N	ammonium benzoate	0.7160	Valium tab1	0.7143	6
Residual	1	Valium tab 1	0.7030	N					
	2	3,5-difluoronitro benzene	0.7972	N	ethidium bromide	0.7772	5-nitrosiso phthalic acid	0.7723	7
Residual	2	2,3-dinitrotoluene	0.7147	N					
Methamphetamine: DMS (60:40)	1	ammonium benzoate	0.7503	N	3-[(benzyloxy carbonyl) amino]	0.7485	(R)-(+)-3-(benzyl oxycarbonyl)-4-	0.7333	7
Residual	1	tri-n-butyl citrate	0.7210	N					
Methamphetamine: DMS (50:50)	1	dimethyl sulfide	0.6741	N	3-methyl-2(3H)-benzothiazolone	0.6484	methyl vinyl sulfone	0.6475	4
Residual	1	terephthalic acid	0.7560	N					
	2	methyl sulfone	0.8188	Y	dichloromethane	0.7238	(S)-(-)-N-(trifluoro acetyl) prolyl chloride	0.6890	3
Residual	2	terephthalic acid	0.7250	N					

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Methamphetamine: DMS (40:60)	1	dimethyl sulfide	0.6635	N	3-methyl-2(3H)-benzothiazolone	0.6576	(1,1-dimethyl propyl) benzene	0.6368	3
Residual	1	terephthalic acid	0.7590	N					
Methamphetamine: DMS (30:70)	1	dimethyl sulfide	0.7335	N	dichloromethane anhydrous	0.6963	ethyl sulfone	0.6907	3
Residual	1	terephthalic acid	0.7450	N					
Heroin: Quinine (80:20)	1	1,7-dimethoxy naphthalene	0.8948	N	zirconium (IV) silicate	0.8920	2-methylthio-1,3-triazole	0.8850	7
Residual	1	tetramethylene sulfoxide	0.7520	N					
	2	ethidium bromide	0.9381	N	triaminoguanidinium dinitropyrazolopyrazole	0.9032	trinitrotoluene (TNT)	0.8933	7
Residual	2	ethidium bromide	0.8520	N					
Heroin: Quinine (60:40)	1	zirconium (IV) silicate	0.9134	N	2-methylthio-1,3-thiazole	0.8805	2-ethyl naphthalene	0.8730	7
Residual	1	terephthalic acid	0.7670	N					
Heroin: Quinine (50:50)	1	2-methylthio-1,3-thiazole	0.8373	N	zirconium (IV) silicate	0.8186	5-methyl quinoxaline	0.8116	7
Residual	1	5-methyl quinoxaline	0.7930	N					
	2	ethidium bromide	0.8907	N	triaminoguanidinium dinitropyrazolopyrazole	0.8347	acridine orange channel	0.8308	3
Residual	2	acridine orange channel	0.8161	N					
Heroin: Quinine (40:60)	1	2-methylthio-1,3-thiazole	0.8982	N	zirconium (IV) silicate	0.8940	4-methoxy-1-naphthol	0.8393	7

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Residual	1	tetramethylene sulfoxide	0.7610	N					
Heroin: Quinine (30:70)	1	zirconium (IV) silicate	0.9185	N	1,7-dimethoxy naphthalene	0.8835	2-methylthio-1,3-triazole	0.8823	7
Residual	1	terephthalic acid	0.7630	N					
Ammonium Nitrate: Sugar (80:20)	1	silver nitrate	0.9751	N	barium nitrate	0.9732	lead nitrate	0.9691	4
Residual	1	terephthalic acid	0.7690	N					
	2	ammonium nitrate	0.9412	Y	samarium (III) nitrate 6H2O	0.9085	thallium(ous) nitrate	0.9033	6
Residual	2	terephthalic acid	0.7890	N					
Ammonium Nitrate: Sugar (60:40)	1	barium nitrate	0.9394	N	silver nitrate	0.9312	lead nitrate	0.9232	4
Residual	1	terephthalic acid	0.7789	N					
Ammonium Nitrate: Sugar (50:50)	1	barium nitrate	0.9684	N	silver nitrate	0.9590	lead nitrate	0.9525	5
Residual	1	terephthalic acid	0.7439	N					
	2	Ethidium bromide	0.7641	N	2,5-pyridine dicarboxylic acid	0.7441	trinitrotoluene (TNT)	0.7366	7
Residual	2	3,4-dinitrotoluene	0.7110	N					
Ammonium Nitrate: Sugar (40:60)	1	barium nitrate	0.9738	N	silver nitrate	0.9650	lead nitrate	0.9595	5
Residual	1	terephthalic acid	0.7440	N					
Ammonium Nitrate: Sugar (30:70)	1	table sugar	0.7149	Y	silver lactate	0.6987	nitropropane	0.6791	3

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Residual	1	tri-n-butyl citrate	0.7350	N					
Ammonium Nitrate: Cumin (80:20)	1	5-methyl quinoxaline	0.7695	N	S-(-)-3,3'-dibromo-1,1'bi-2-napthol	0.7296	ethidium bromide	0.7274	7
Residual	1	5-methyl quinoxaline	0.7680	N					
	2	E-thiocaprolactam	0.6773	N	2-Nitro-N-methyl benzylamine	0.6695	2-hydroxy-4-methyl quinoline	0.6369	7
Residual	2	E-thiocaprolactam	0.6770	N					
Ammonium Nitrate: Cumin (60:40)	1	5-methyl quinoxaline	0.7227	N	pyridoxine HCl	0.7203	acridine orange channel	0.7142	7
Residual	1	pyridoxine HCl	0.7190	N					
Ammonium Nitrate: Cumin (50:50)	1	tri-n-butyl citrate	0.6094	N	acridine orange channel	0.6055	x	x	x
Residual	1	tri-n-butyl citrate	0.6090	N					
	2	ethidium bromide	0.7496	N	acridine orange channel	0.7363	2,3,4-trifluoro nitrobenzene	0.7052	7
Residual	2	acridine orange channel	0.7180	N					
Ammonium Nitrate: Cumin (40:60)	1	5-methyl quinoxaline	0.6780	N	1-(-2-bromoethyl) naphthalene	0.6303	2,3-dichloro benzaldehyde	0.6267	4
Residual	1	5-methyl quinoxaline	0.6770	N					
Ammonium Nitrate: Cumin (30:70)	1	5-methyl quinoxaline	0.7865	N	pyridoxine HCl	0.7254	S-(-)-3,3'-dibromo-1,1'-bi-2-napthol	0.6959	7
Residual	1	5-methyl quinoxaline	0.7520	N					
SPECIFICITY									

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
d,l-amphetamine sulfate	1	sodium tartrate dibasic 2H2O	0.7448	N	2,9-dimethyl-4,7-diphenyl-1,10	0.7106	(R)-3,3'-bis(triphenyl silyl)-1,1'-bi-2-naphthol	0.6936	7
MDMA	1	piperonylamine	0.7265	N	4-bromo-3-nitroanisole	0.7261	piperonyl acetate	0.7178	7
MDA	1	ethidium bromide	0.7669	N	trinitrotoluene (TNT)	0.7443	triaminoguanidinium dinitropyrazolopyrazole	0.7384	7
MDEA	1	hydroquinine	0.7314	N	(+)-cinchonine	0.7312	S(-)-alpha-methyl-1-naphthalenemethanol	0.7163	7
morphine sulfate	1	acridine orange channel	0.7718	N	3,4-dinitrotoluene	0.7260	ethidium bromide	0.7024	6
codeine sulfate	1	vinyl chloride 90% vinyl acetate 10%	0.6721	N	(R)-(+)-2-Acetoxy succinic anhydride	0.6554	Ethyl thioacetate	0.6366	4
benzocaine	1	ethyl 4-aminobenzoate	0.9640	Y	dichloromaleic anhydride	0.9327	ethyl 4-(butylamino) benzoate	0.9121	4
lidocaine	1	sodium tartrate dibasic 2H2O	0.6432	N	4,4'-azobis(4-cyanovaleric acid)	0.6185	S(-)-alpha-methyl-1-naphthalene MeOH	0.6178	3
procaine	1	4-butoxy benzaldehyde	0.7598	N	methyl 4-acetamido-5-chloro-2	0.7537	p-anisaldehyde	0.7526	6
acetylsalicylic acid (ASA)	1	acetylsalicylic acid 99%	0.8977	Y	2-bromofluorene	0.7541	N,N'-B,5(3-methylphenyl-N,N'	0.7395	3
Residual	1	terephthalic acid	0.7420	N					
ibuprofen	1	hydroxybutyric acid	0.8704	N	ibuprofen_CVS junior strength	0.7763	6-(trifluoromethyl) pyridine-3-methanol	0.7665	7
guaifenesin	1	guaiacol glycyryl ether	0.8137	Y	calcium nitrite solution	0.6774	4-bromoveratrole	0.6479	6

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
diphenhydramine	1	hexaphenyl cyclotrisiloxane	0.9043	N	QuadraPure ™ AEA	0.9036	hydratop aldehyde	0.8974	7
chlorpheniramine	1	dipyridamole	0.7386	N	2,9-dimethyl-4,7-diphenyl-1,10-	0.7170	B-naphthol	0.7154	7
pseudoephedrine	1	promethazine	0.9070	N	phenol, polymer bound	0.8278	o-benzyl-6-serine	0.8206	7
Dimethyl sulfone (DMS)	1	dimethyl sulfone	0.9266	Y	dichloromethane	0.7628	5-(-)-N-(Trifluoroacetyl) prolyl chloride	0.7370	4
Baking soda	1	ammonium nitrate	0.8778	N	samarium (III) nitrate 6H2O	0.8745	ammonium carbonate	0.8552	5
Acetaminophen (ACE)	1	acetaminophen	0.9175	Y	phenacetin	0.8075	4'-aminoacet-aniline	0.7859	1
Residual	1	tetramethylene sulfoxide	0.7500	N					
urea	1	calcium sulfate dihydrate	0.9266	N	guanidine	0.9254	pyridine HCl	0.9159	5
ferric nitrate	1	yttrium (III) nitrate 6H2O	0.9520	N	lanthanum (III) nitrate hydrate	0.9468	Barium nitrate	0.9466	7
sodium perborate	1	K Na tartrate 4H2O	0.6410	N	L-proline	0.6267	Potassium sodium tartrate	0.6027	1
fertilizer (13% total N) prills	1	lead styphnate	0.7705	N	2-methyl-4' nitroaniline	0.7638	4-Nitroaniline	0.7149	7
Residual	1	lead styphnate	0.7230	N					
fertilizer (13% total N) ground	1	lead styphnate	0.8182	N	lanthanum Iodide	0.7779	2,4-dinitrophenyl hydrazine	0.7770	6
Residual	1	N,n-ethyl-N-2-nitroxy ethyl) nitramine	0.6900	N					
Turmeric : cardamom (50:50)	1	ethidium bromide	0.8630	N	B-naphthol	0.8572	triaminoguanidinium dinitropyrazolopyrazole	0.8427	7

Sample	Trial	Match (1)	Hit Quality (1)	Correct? Y/N	Match (2)	Hit Quality (2)	Match (3)	Hit Quality (3)	# other hits
Residual	1	B-naphthol	0.8390	N					
sodium hydroxide (lye)	1	4-nitro-phenylene diamine	0.8183	N	2-amino-5-nitropyridine	0.8147	trithiocyanuric acid	0.7742	6
sulfuric acid	1	sulfuric acid (conc.)	0.9481	Y	phosphoric acid	0.9143	hydrophosphorous acid	0.8817	3
ammonium hydroxide	1	3,4-dinitrotoluene	0.6706	N	2,3-dinitrotoluene	0.6612	2'-Deoxyguanosine 5'-monophosphate	0.6271	7
citric acid	1	sodium phosphate tribasic	0.6101	N	x	x	x	x	x