Technical Evaluation:

Rigaku Analytical Devices Progeny™ ResQ™

Application: Illegal Drug Screening

Device: Progeny™ ResQ™ , Manufactured by Rigaku Analytical Devices

Hardware Serial Number: P15110125

Software Version: 1.3.0.1

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Edward G. Bartick, Biographical Sketch

Edward Bartick is a research professor at the George Washington University Department of Forensic Sciences who is involved in the development of forensic analytical methods of materials. He completed a Ph.D. at the Institute of Materials Science in 1978 at the University of Connecticut. He has worked for Perkin-Elmer Corp. and Spectra-Tech, Inc. as a senior infrared spectroscopy applications chemist and has supervised an analytical materials research group for Raymark Corporation. In 1986, he joined the FBI Laboratory as a research scientist in forensic methods development. In 1991 he started the one week class, "Infrared Spectrometry for Trace Analysis" for forensic examiners. He acted as research advisor for Ph.D. and MS graduate students from the University of Virginia, Virginia Tech, and The George Washington University while they worked on forensic vibrational spectroscopy thesis projects in Dr. Bartick's laboratories at the FBI Academy. January 2007 Dr. Bartick retired from the FBI to direct the Forensic Science Program at Suffolk University in Boston where he expanded the curriculum. He returned to the Washington, DC area to join GWU as a research professor in the fall of 2013.

Over the course of Dr. Bartick's career, he has developed analytical methods from quantitative field analysis of street drugs to non-invasive infrared spectral imaging of latent finger prints including the identification of trace materials imbedded within the ridge patterns. His studies have included the analysis of explosives and illicit drugs with hand held IR and Raman spectrometers. His consulting led Ahura Scientific (now a part of Thermo Fisher Scientific) to the development of one of the most successful hand held instrument software strategies in the industry. He was involved with stand-off passive IR in the early years for the detection of clandestine drug manufacture. With infrared and Raman spectroscopy, he has developed forensic analysis of single fibers, pressures sensitive adhesive tapes, inks, copy toners, paints and biological warfare agents. In the pursuit of the cutting edge of forensic analysis, his current research involves the development of statistical significance of class evidence and the development of hand-held optical spectrometers for field and laboratory applications using multivariate statistical analysis.

Dr. Bartick has authored 60 technical publications, including 11 book chapters. He was awarded the FBI Director's Award in 1994 and 1996. In 1994 he founded the Scientific Working Group for Materials Examination (SWGMAT). He chaired the group through 1997 and continued to play an active role as chair of the Database Subgroup until spring of 2014 when the Organization *of Scientific Area Committees* (*OSAC*) at NIST assumed the role of SWGs. Dr. Bartick is a Fellow of the American Academy of Forensic Sciences, a charter member of American Society of Trace Evidence Examiners (ASTEE), a member of the American Chemical Society and the Society for Applied Spectroscopy.

Introduction:

Forensic drug analysis laboratories typically have the heaviest workload in crime laboratories. The Baltimore County Police Department, Forensic Services Section (BCPD-FSS), has estimated the drug evidence submitted to the laboratory to be approximately 60% of the total evidence submissions. Upon analysis of the evidence, approximately 20% result in court submission. The laboratory analytical methods are time consuming and expensive equipment is required. There is interest in the potential of using a portable Raman spectrometer to screen the samples at precincts prior to formal submission. Because of the fast and simple analysis of the Rigaku Analytical Devices, Progeny ResQ Raman spectrometer, this could result in considerable time and money savings to the laboratory. With the success of this screening approach, the return on investment (ROI) would be significant and would be of great interest to forensic drug laboratories throughout the world. Additionally, the spectrometer could be used in the field to determine if arrest is warranted. With accurate results, this could insure the reason for arrest and alleviate the problems encountered with incorrect inappropriate arrests.

The objective of the study was to evaluate the performance of Progeny ResQ to identify illegal drugs using two proprietary detection algorithms: Wavelet and Rigaku Mixtures. Wavelet is Rigaku Analytical Devices' proprietary ID algorithm that identifies the most spectroscopically prominent component of an unknown sample. The Rigaku Mixture algorithm will identify pure compounds as single components, but will automatically detect the presence of a mixture and identify the other components.

Product Specifications:

Progeny ResQ identifies chemicals using Raman spectroscopy, which collects a chemical signature of a sample that results from the inelastic scatter from an excitation laser. Progeny ResQ uses a 1064 nm diode laser, adjustable between 30 and 490 mW. By using excitation at 1064 nm, fluorescence interference is minimized, which allows for analysis of a wider range of compounds, including many colored substances. The Raman signal is measured on a 512 pixel indium gallium arsenide (InGaAs) detector and is assembled into a spectrum. After analysis, the sample's chemical signature is searched against an onboard library database to identify the sample. The library onboard Progeny ResQ at the time of this study had over 12,500 compounds including controlled substances, cutting agents, OTC medications, chemical precursors, explosives, chemical weapons, and toxic substances. Data are saved as .pdf, .txt, xml (convertible to .spc).

Progeny ResQ weights approximately 3.5 lbs (1.6 kg) and measures approximately 11.8 x 3.2 x 2.9 inches (29.9 x 8.1 x 7.4 cm). The instrument is rated IP 68, and has passed numerous MILSTD810G tests for durability (e.g. High/low storage temperature, High/Low Operating Temperature, Thermal Shock, Mechanical Shock, Vibration, Immersion, Humidity, Cargo Drop). The instrument comes packed in a rugged Pelican case, with two batteries (each with 6+ hour battery life), A/C power adapter, USB Cable, adjustable focus nose cone, certified calibration standard, and a sampling accessory that hold vials, tablets, and baggies securely against the instrument during analysis. The

unit also has various sampling accessories, docking station, and a belt/shoulder holster available as options for purchase.

Workflow

When Progeny ResQ is powered on, the user is taken to a main screen where the operator can initiate a new scan, view old results files (organized by day/week/month), or change instrument settings (if they have the appropriate administrator credentials). The user can initiate a scan by using either the touch screen or three pushes of the physical buttons. If running the instrument using the autocollect feature (default), laser power, exposure time, and number of averages are automatically optimized based on a test pulse. Advanced users can manually select these parameters if desired. The entire analysis process, starting from the main screen takes approximately 15-25 seconds for the samples analyzed in this study.

Results Display and Secure Reports

The results are displayed on a screen with either a red or green header, which indicate whether or not the identified result is a threat or not. In addition to the identified substance, the results screen also displays synonyms/common names, classification, and hazard information. At this time, a tamper proof date and time stamped pdf report is automatically generated, which displays all spectroscopic parameters, file information, chemical signature, and library search parameters. Following analysis of an unknown substance, the user can capture an image of the sample or crime scene using the onboard 5 MP digital camera. Any pictures taken of the sample and/or crime scene are attached to the pdf report. All spectroscopic data, reports, and picture files can be synced to an external computer via USB or device-to-device WiFi connection (which can also be disabled if desired). Although not evaluated in this study, the user can simultaneously sync data to a computer and recharge the battery by dropping the unit into a docking station, which is an available option.

Samples Analyzed with Progeny ResQ Spectrometer (160 total analyses)

A. Pure Standards: Cover a range of illegal drug types:

List of pure samples run (the samples were all certified U.S.P. as are the library standards) with abbreviations in brackets if used

1. Cocaine
2. Cocaine Base
3. Heroin
4. 3,4-Methylenedioxy-methamphetamine (Ecstasy) [MDMA]
5. Mephedrone HCl [Meph]
6. Methamphetamine HCl [Meth]
7. 3, 4 Methylenedioxypyrovalone HCl [MDP]
8. 5F-PB-22
9. STS-135
10. -(S) Cathione HCl Diphenhydramine (Crushed Pill) [Cath]
11. Diphenhydramine (Crushed Pill) [DPHD]

B. Street Samples: Evaluate the performance of the instrument against real world materials.

List of Street Samples:

1. Cocaine
2. Cocaine Base
3. Heroin
4. MDMA
5. Case Sample that had been misidentified as cocaine in the field, but was later found to be a benign substance when GC-MS was used

Progeny ResQ Analysis Methodology:

All spectra were collected using the Autocollect feature, which automatically optimizes laser power and observation time. All searches were against the Master Library, which was comprised of more than 12,500 compounds at the time of the study.

Pure samples were scanned through glass containers by holding the spectrometer snugly to the edge. The quantity of the samples was at on the order of 5-10 mg. Ten trials were performed for all pure compounds. The instrument was repositioned between trials.

Case samples (street drugs) were previously analyzed and identified using GC-MS at the Baltimore County Police Department, Forensic Sciences Services. The amount of material available for follow-on analysis using Progeny ResQ after analysis by GC-MS was on the order of 10 milligrams. The samples were scanned through glass vials in the same manner as pure standards. Because diluents are often placed in street samples, the potential of heterogeneity exists. Therefore, 10 trials for each sample (instrument repositioned between trials) were taken to test whether sample heterogeneity would be reflected in the results. All results were tabulated for convenient comparison.

Results :

1, Pure Samples of Illegal Drugs

All trials of all samples were identified with 100% accuracy with both Wavelet and Rigaku Mixture algorithms. No mixture components were reported as one would expect for pure compounds.

Table 1. Pure Sample Results with the Use of the Rigaku Wavelet algorithm

Sample Name	Trial 1	Trial 2	Trial 3	Trial 4	Trial 5	Trial 6	Trial 7	Trial 8	Trial 9	Trial 10
Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine
Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base
Heroin	Heroin	Heroin	Heroin	Heroin	Heroin	Heroin	Heroin	Heroin	Heroin	Heroin
MDMA	MDMA	MDMA	MDMA	MDMA	MDMA	MDMA	MDMA	MDMA	MDMA	MDMA
Meph	Meph	Meph	Meph	Meph	Meph	Meph	Meph	Meph	Meph	Meph
Meth	Meth	Meth	Meth	Meth	Meth	Meth	Meth	Meth	Meth	Meth
MDP	MDP	MDP	MDP	MDP	MDP	MDP	MDP	MDP	MDP	MDP
5F-PB-22	5F-PB-22	5F-PB-22	5F-PB-22	5F-PB-22	5F-PB-22	5F-PB-22	5F-PB-22	5F-PB-22	5F-PB-22	5F-PB-22
STS-135	STS-135	STS-135	STS-135	STS-135	STS-135	STS-135	STS-135	STS-135	STS-135	STS-135
Cath	Cath	Cath	Cath	Cath	Cath	Cath	Cath	Cath	Cath	Cath
DPHD	DPHD	DPHD	DPHD	DPHD	DPHD	DPHD	DPHD	DPHD	DPHD	DPHD

Table 2. Pure Sample Results with the Use of the Rigaku Mixture algorithm

Sample Name	Trial 1	Trial 2	Trial 3	Trial 4	Trial 5	Trial 6	Trial 7	Trial 8	Trial 9	Trial 10
Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine
Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base
Heroin	Heroin	Heroin	Heroin	Heroin	Heroin	Heroin	Heroin	Heroin	Heroin	Heroin
MDMA	MDMA	MDMA	MDMA	MDMA	MDMA	MDMA	MDMA	MDMA	MDMA	MDMA
Meph	Meph	Meph	Meph	Meph	Meph	Meph	Meph	Meph	Meph	Meph
Meth	Meth	Meth	Meth	Meth	Meth	Meth	Meth	Meth	Meth	Meth
MDP	MDP	MDP	MDP	MDP	MDP	MDP	MDP	MDP	MDP	MDP
5F-PB-22	5F-PB-22	5F-PB-22	5F-PB-22	5F-PB-22	5F-PB-22	5F-PB-22	5F-PB-22	5F-PB-22	5F-PB-22	5F-PB-22
STS-35	STS-35	STS-35	STS-35	STS-35	STS-35	STS-35	STS-35	STS-35	STS-35	STS-35
Cath	Cath	Cath	Cath	Cath	Cath	Cath	Cath	Cath	Cath	Cath
DPHD	DPHD	DPHD	DPHD	DPHD	DPHD	DPHD	DPHD	DPHD	DPHD	DPHD

2, Case Samples (street drugs, varying purity)

Wavelet Algorithm

As shown in Table 1, all samples and all the trials resulted in 100% the same identification as the GC-MS identification during regular case analysis.

Table 3. Pure Sample Results with the Use of the Rigaku Wavelet algorithm

Case Sample Analysis Identification	Trial 1	Trial 2	Trial 3	Trial 4	Trial 5	Trial 6	Trial 7	Trial 8	Trial 9	Trial 10
Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Not Done
Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base
Heroin	Heroin	Heroin	Heroin+	Heroin	Heroin	Heroin	Heroin	Heroin	Heroin	Heroin
MDMA	MDMA	MDMA	MDMA	MDMA	MDMA	MDMA	MDMA	MDMA	MDMA	MDMA
Magnesium Sulfate	Magsulf	Magsulf	Magsulf	Magsulf	Magsulf	Magsulf	Magsulf	Magsulf	Magsulf	Magsulf

Use of the Rigaku Mixture algorithm

All samples had the same illicit component identified as was reported in the GC-MS analysis during regular case analysis. In three of the five street samples, additional components were detectable in the results obtained on Progeny ResQ. Table 4. shows the results from the ten trials for the five street samples analyzed. The components are listed in order that they were reported by the software.

Table 4. Street Sample Results with the Use of the Rigaku Mixture algorithm

Case Sample Analysis Identification	Trial 1	Trial 2	Trial 3	Trial 4	Trial 5	Trial 6	Trial 7	Trial 8	Trial 9	Trial 10
Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Cocaine	Not Done
Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base	Cocaine Base
Heroin	Heroin+ Tylenol	Heroin+ Acetam	Heroin+ Ethylen	Heroin+ Acetam	*Heroin+* Ethylen	Heroin+ Ethylen	Heroin+ Ethylen	Heroin+ Ethylen	Heroin+ Ethylen	Heroin+ Ethylen
MDMA	PMK + SST + MDMA	MDMA + D-R	PMK + SST + MDM A	SST + MDMA	SST + MDMA	MDMA + D-R	PMK + SST + MDMA	MDMA + D-R	MDMA	PMK + SST + MDMA
Magnesium Sulfate	Magsulf + SST	Magsulf	Magsulf	Magsulf	Magsulf	Magsulf + D-R	Magsulf + SST	Magsulf + SST	Magsulf	Magsulf

Abbreviations:
Tylenol = Tylenol - Cold and Flu
Acetom = Acetaminophen Tablet
Ethylen = Ethylenedianline
PMK = Pyperonal Methyl Ketone
SST = Sodium Stannate (IV) Trihydrate
D-R = D-Ribose 1-13C
Magsulf = Magnesium Sulfate Heptahydrate

Summary of Results:

- For the pure samples, the 100% accuracy is expected, because all the samples were listed in the library. As one would expect for pure compounds, no mixture components were reported in the search results.
- The accuracy of the Wavelet algorithm results were 100% matches with the case identified component in street samples. Thus, clearly demonstrating the ability to pick the main component while spectral interferences of other components exist.
- The Mixture algorithm produced 100% matches with the case identified component, while identifying other components that exist in the sample.
- During the trials of the street samples, multiple trials showed that there is definitely inhomogeneity in certain sample. However, the main component was consistently identified as present.
- The sample that was falsely considered a drug and brought into the lab for analysis was quickly identified as magnesium sulfate by Progeny ResQ. Had this unit been used to scan incoming material, time, effort and money would have been saved by avoiding costly GC-MS lab analysis.