# Pocket-Size Near-Infrared Spectrometer for Narcotic Materials Identification



Next-Generation Spectroscopic Technologies VII, edited by Mark A. Druy, Richard A. Crocombe, Proc. of SPIE Vol. 9101, 91010O · ©2014 SPIE · CCC code: 0277-786X/14/$18 · doi: 10.1117/12.2050019

# Pocket-Size Near-Infrared Spectrometer for Narcotic Materials Identification

Christopher G. Pederson[a *], Donald M. Friedrich[a], Chang Hsiung[a], Marc von Gunten[a], Nada A. O'Brien[a], Henk-Jan Ramaker[b], Eric van Sprang[b], Menno Dreischor[b]
[a]JDSU Corporation, Santa Rosa, California, USA 95407
[b]Toegepaste Industriële Procesbeheersing (TIPb), Amsterdam, The Netherlands

## ABSTRACT

While significant progress has been made towards the miniaturization of Raman, mid-infrared (IR), and near-infrared (NIR) spectrometers for homeland security and law enforcement applications, there remains continued interest in pushing the technology envelope for smaller, lower cost, and easier to use analyzers. In this paper, we report on the use of the MicroNIR Spectrometer, an ultra-compact, handheld near infrared (NIR) spectrometer, the, that weighs less than 60 grams and measures < 50mm in diameter for the classification of 140 different substances most of which are controlled substances (such as cocaine, heroin, oxycodone, diazepam), as well as synthetic cathinones (also known as bath salts), and synthetic cannabinoids. A library of the materials was created from a master MicroNIR spectrometer. A set of 25 unknown samples were then identified with three other MicroNIRs showing: 1) the ability to correctly identify the unknown with a very low rate of misidentification, and 2) the ability to use the same library with multiple instruments. In addition, we have shown that through the use of innovative chemometric algorithms, we were able to identify the individual compounds that make up an unknown mixture based on the spectral library of the individual compounds only. The small size of the spectrometer is enabled through the use of high-performance linear variable filter (LVF) technology.

**Keywords:** Narcotics, explosives, illicit substances, near infrared, miniature spectrometer, linear variable filter, handheld spectrometer

## 1. INTRODUCTION

The optical and infrared spectroscopy industry is undergoing a major transformation. Much-akin to the computer industry, the size and weight of the instruments are shrinking from bench-top size to pocket-size. Overall system costs are decreasing, and the performance continues to move from 'good-enough' to approaching some aspects of bench-top performance. These miniature handheld spectrometers are enabling a new population of users taking measurements in the field by non-technical individuals whereby historically these tests have been conducted in the laboratory by highly skilled technicians. The tests are non-destructive and take only a few seconds to complete, enabling the capability for real-time results leading to more efficient decision making. Because of the ease of use and low cost of these new miniature devices, increasing interest is being seen in areas of law enforcement and hazardous material responders.

Police officers, border patrol agents, first responders or military personnel could use a miniature spectrometer to analyze suspicious substances that may be suspected illegal or lethal.

In this paper, we report on the performance of the world's smallest, fully contained (detector, light source, collection optics, dispersing element and control and readout electronics) NIR spectrometer, the MicroNIR™ Spectrometer, to establish the viability of using the device to correctly classify common illicit substances, confusants and explosives. The MicroNIR spectrometer is powered and controlled with a smart mobile device, such as a tablet, phablet, or a smartphone.

*Corresponding author: chris.pederson@jdsu.com

Next-Generation Spectroscopic Technologies VII, edited by Mark A. Druy, Richard A. Crocombe,
Proc. of SPIE Vol. 9101, 91010O · © 2014 SPIE · CCC code: 0277-786X/14/$18 · doi: 10.1117/12.2050019

The National Forensic Science Technology Center (NFSTC) in Largo, FL was tasked to collect a library of spectral scans to evaluate the potential of the MicroNIR miniature spectrometer for forensic identification of controlled substances, diluents, pharmaceuticals and other chemicals. Near infrared spectroscopy is a non-destructive and confirmatory technique that can be implemented to identify a variety of forensics samples. Traditionally, it is equipment that is limited to a laboratory environment, but the handheld and miniature design of the MicroNIR, without the limitations of moving parts, opens this technology to non-traditional environments such as law enforcement and first responders.

This research was conducted into two phases; 1) a library development phase and 2) a conformity analysis of the developed calibration and performance evaluation across three different MicroNIR spectrometers.

Phase I consisted of the scanning of a large number of drug and drug-related compounds in order to build a classification library which includes the top drugs reported by forensic laboratories as published in the DEA sponsored NFLIS report of 2010 [1]. Additional controlled substances and pharmaceuticals were included, as well as precursors, diluents and other common chemicals.

Phase II of the testing occurred after the initial data analysis and classification algorithms were developed at JDSU. NFSTC assessed the MicroNIR for accuracy (conformity) using a sub-set of 25 previously run samples. The three spectrometers used for phase two included the original instrument used for calibration development (Serial number S1-2012-0048T) and two new production units (Serial numbers S1-00129 and S1-00138).

In a separate study, researchers at Toegepaste Industriële Procesbeheersing (TIPb) in Amsterdam, The Netherlands, developed models for identifying controlled substances that are present in street drugs. The models relied on scans and libraries of pure compounds only.

## 2. SPECTROMETER, EXPERIMENTAL DESIGN & SETUP

### 2.1 Spectrometer

The MicroNIR spectrometer is a disruptive and enabling miniature spectrometer designed to measure diffuse reflection spectra in the NIR region of the electromagnetic spectrum to be used for real-time, point-of-use NIR chemometrics applications. The MicroNIR owes its small size to the novel thin-film linearly variable filter (LVF) used as the dispersive element versus traditional diffraction based spectrometers. The LVF is a dielectric thin-film Fabry-Perot bandpass filter deposited using energetic processes, well-known to produce stable and reliable optical components [2]. The MicroNIR is seen in Figure 1 and further details as to the spectrometer design theory have been previously presented [3].

Figure 1: The MicroNIR spectrometer.

The LVF filter coating used in the MicroNIR is intentionally wedged in one direction. Since the center wavelength of the bandpass filter is a function of the coating thickness, the peak transmitted wavelength varies continuously along the direction of the wedge. This working principle is illustrated in Figure 2.

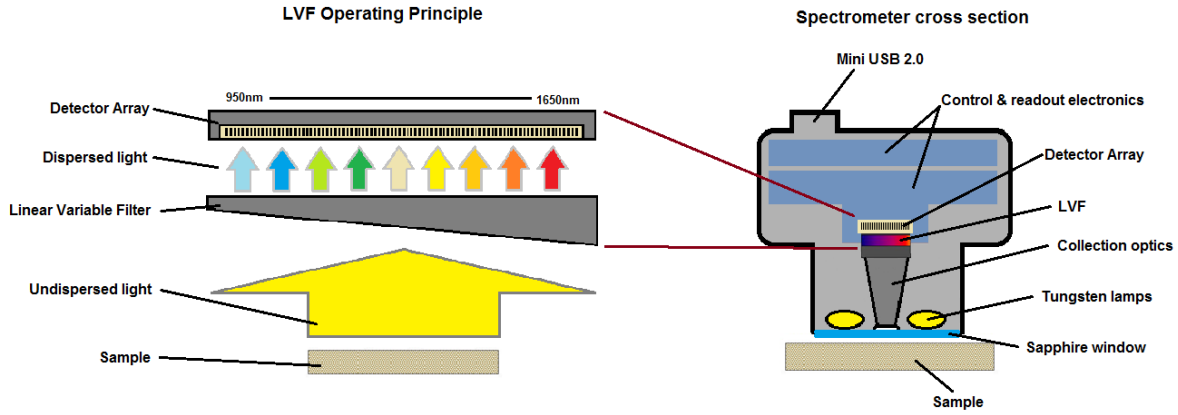


Figure 2: An illustration of the optical design and cross section of the MicroNIR operated in diffuse reflection mode.

Key attributes of the MicroNIR 1700 spectrometer are summarized in Table 1. For applications in point-of-use and process analytical technology (PAT), measurement reproducibility among multiple MicroNIR spectrometers as well as repeatability of measurements on each MicroNIR are well understood and documented in a previously published article [4].

Table 1: Key performance attributes of the MicroNIR 1700 spectrometer.

| | |
|---|---|
| Weight | 60 grams |
| Dimensions | 45mm diameter x 42mm height |
| Spectral Range | MicroNIR 1700: 950-1650nm |
| Number of pixels | 128 pixels, 125 point standardized grid |
| Optical Resolution | <1.25% of center wavelength, i.e. at 1000nm wavelength, resolution is <12.5nm |
| Geometric Resolution | 6.25nm per pixel |
| Wavelength Accuracy | < 3 nm, as compared to NIST SRM-2036 |
| Wavelength Repeatability | < 1 nm, as compared to NIST SRM-2036 |
| Power Requirement | USB powered, <500mA at 5V |
| Operating Temperature | -20°C to 40°C |

## 2.2 Sample presentation & data acquisition

One of the challenges in measuring street narcotics is that the sample size is very small. Thispresents challenges for many analytical technologies. To increase the probability of success, a reproducible sampling protocol and presentation capable of accommodating a wide range of material volumes was investigated and subsequently developed. The final sample presentation that yielded the highest reproducibility across sample volumes was the use of a polyethylene bag with an X heat sealed onto the bag creating a symmetrical pocket. This ‘X-bag’ can be seen below in Figure 3.

Figure 3: Sample in 'X-bag' and placement on the MicroNIR

One hundred and forty (140) compounds were scanned at NFSTC with the MicroNIR 1700 using the windowed collar sampling accessory which contains an integrated sapphire window to maintain a consistent sample-to-spectrometer distance. A 99% diffuse reflectance panel was utilized as the spectrometer's 100% reference value. The system 'zero' was collected with no sample in the spectrometer field of view. An integration time of 9ms and a spectrum averaging of 50 was used for all spectral acquisitions. Spectrum averaging refers to the number of single scans averaged together to represent a single spectrum acquisition. Spectrum averaging seeks to improve overall spectrum signal-to-noise ratio.

The samples were transferred into the 'X-Bags' and the 99% reflectance panel was placed on top of the sample X-bag to serve as a backer to mitigate any light loss. The use of the backer serves to boost the overall measurement signal-to-noise on a small volume sample. Some of the materials measured were dark in color. For these materials, the instrument 100% reference values were collected using both a 99% & 50% diffuse reflectance panel. Use of the 50% reference panel seeks to maximize the spectral characteristics of the dark materials. For each of the 140 materials, 5 replicate scans were collected to account for any sampling and sample volume variation.

Following data acquisition, the spectra were imported into The Unscrambler® X software version 10.2 manufactured by CAMO Software AS in Woodbridge, NJ for spectral analysis and calibration model development.

After the development of a predictive calibration model, additional conformity spectra were collected on three different MicroNIR spectrometers to serve as a test set for model performance. 25 samples of the original 140 were scanned at a later date from the original calibration data acquisition. Three spectrometers were used to investigate direct calibration transfer where the model is deployed on data from a different spectrometer without any data manipulation.

## 3. RESULTS & DISCUSSION

### 3.1 Data Pretreatment

The spectra for this study were collected in diffuse reflection mode and subsequently transformed to absorbance. Spectral variation was witnessed and was believed to be dominated by baseline shifts as a result of sample placement on the spectrometer. As a result, a Savitzky-Golay 1$^{st}$ derivative (5 point smoothing) was applied first to accentuate small changes in the spectra followed by a Standard Normal Variate (SNV) correction to minimize the baseline variances resulting from sample volume variances in the X-bags. Both data pretreatments are commonly used with NIR spectra [5]. Figures 4 and 5 below show the pre- and post-treated spectra.

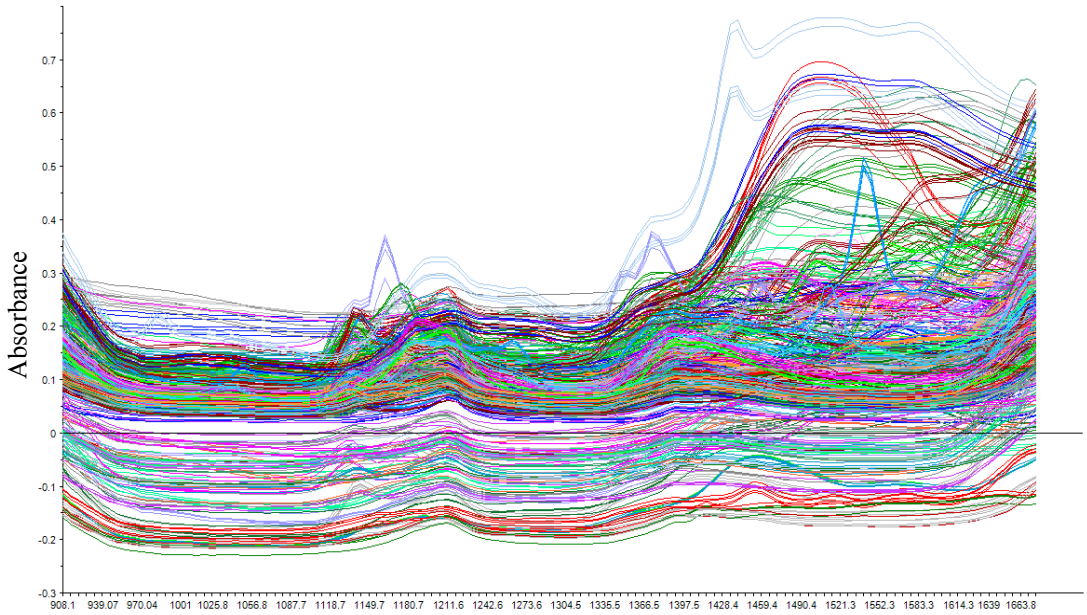


Figure 4: Untreated absorbance spectral dataset

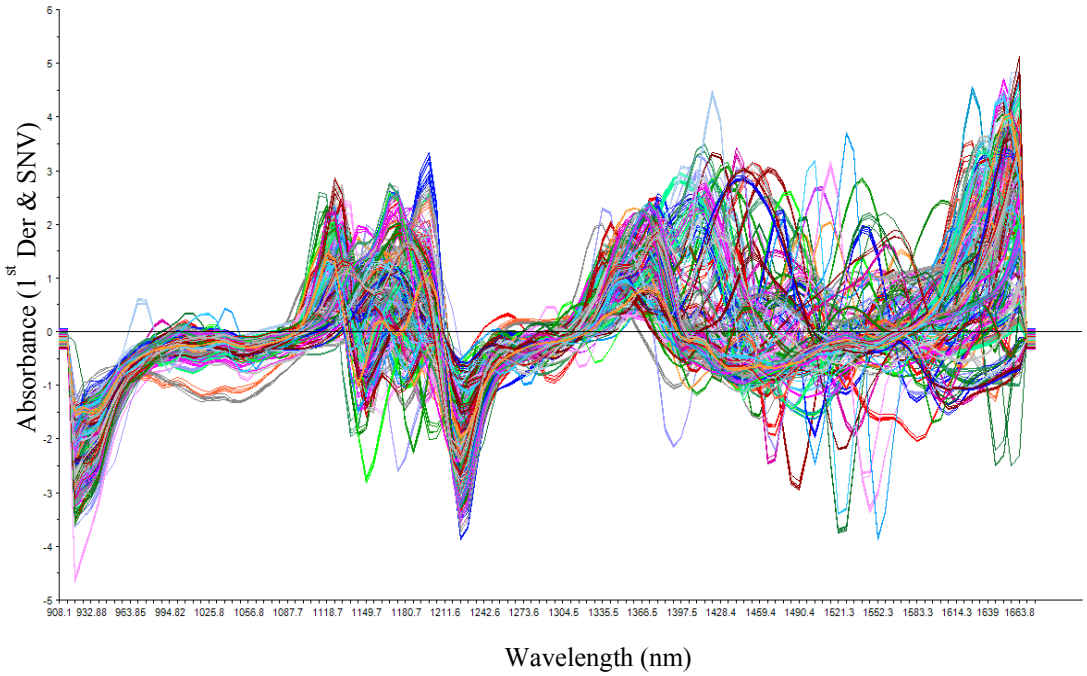


Figure 5: Savitzky-Golay 1st Derivative and Standard Normal Variate treatment of spectral dataset

From the plot of transformed data in Figure 5, one can see that the baseline variability is minimized, and substance-specific features in the spectra are further enhanced.

### 3.2 Principal Component Analysis (PCA) analysis

A Principal Component Analysis (PCA) was performed on the treated spectra to understand how the various materials differentiated between each other as well as understand the spectral repeatability of the within-sample replicate spectral acquisitions. The results of this PCA analysis are seen in the 2-D score plot in Figure 6. The PCA plot shows there is in fact grouping of samples as well as the apparent separation of all materials. In addition to the sample grouping, there also appears to be regional clustering with chemically similar materials such as hormones, cannabinols, and others. These results, though requiring further performance validation, suggest the strong likelihood of success in distinguishing among these materials.

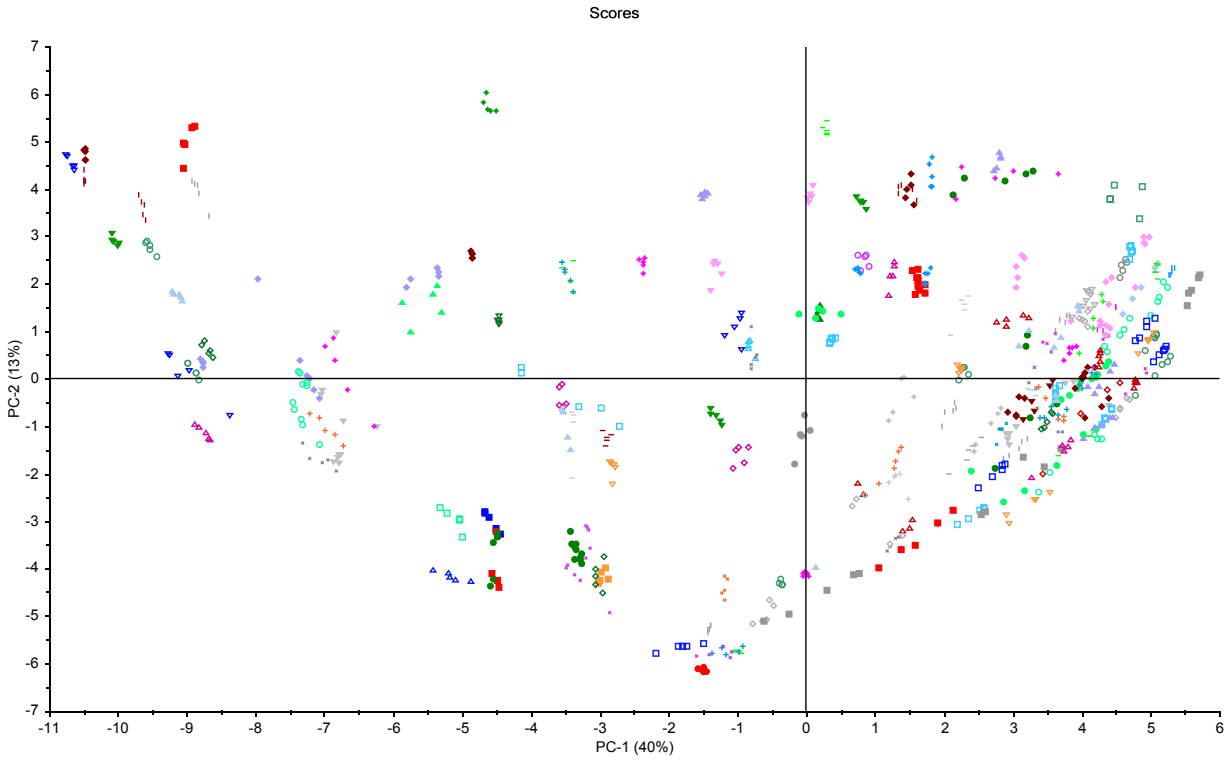


Figure 6: Principal Component Analysis 2-D score plot of pre-treated spectral dataset

### 3.3 Support Vector Machine (SVM) Classification

Support Vector Machine (SVM) is a linear classifier that selects a hyper-plane based on maximizing the separation margin between classes. Its solution only depends on a small subset of training examples (support vectors). And it can be easily extended to nonlinear separation through the kernel machines scheme [6].

SVM has the advantage that it can handle datasets that are multimodal or heterogeneously structured in each of its classes. With its kernel mapping technique, SVM can incorporate prior knowledge into the spectral modeling. Unlike some classifiers that need to adjust parameters for every class in the model (e.g. PC factors and prediction thresholds for SIMCA (Soft Independent Modeling of Class Analogy)), there are only one to two parameters which need to be adjusted and in many cases the default settings are sufficient. Use of a limited set of adjustable parameters aims to prevent models from over-fitting and also shortens the overall model generation time. This has also been shown to demonstrate superb calibration transfer results through its great generalization capability.

The spectral dataset was processed using the Linear C-SVM (classification SVM) algorithm in the Unscrambler software. The resulting classification model of the 140 different compounds yielded a 99.75% training set self-prediction accuracy and a 99.76 % training set cross validation accuracy (where a percentage of training set samples were set aside as prediction set and the remaining samples used to build model and this process continued for hundreds of times and the average prediction success rate was then reported).

### 3.4 Conformity testing

Following the development of the SVM classification model, the subset of 25 samples was predicted for material conformity. The resulting 125 spectra were processed through the calibration model and the prediction results are summarized below in Table 2 for the master calibration instrument (serial number S1-2012-0048T). One misclassification occurred showing an accuracy of 96%, but upon further evaluation of the misclassified spectra, the absorbance values are well outside of the model calibration set indicating an error in spectral acquisition. The final result is a 24/24 classification accuracy yielding 100% accuracy.

Table 2: Prediction results for master calibration MicroNIR serial number S1-2012-0048T.

| Unknown File ID | Predicted | Known ID | Match |
|---|---|---|---|
| 0048T_01_1 | Diltiazem_HCl | Diltiazem HCl | Yes |
| 0048T_02_1 | Inositol | Inositol | Yes |
| 0048T_03_1 | Niacinamide | Niacinamide | Yes |
| 0048T_04_1 | Procaine_HCl | Procaine HCl | Yes |
| 0048T_05_1 | Pseudoephedrine_base | Pseudoephedrine base | Yes |
| 0048T_06_1 | d,l-Amphetamine_sulfate | D,l-amphetamine sulfate | Yes |
| 0048T_07_1 | Carisoprodol | Carisoprodol | Yes |
| 0048T_08_1 | Cocaine_HCl | Cocaine HCl | Yes |
| 0048T_09_1 | Hydromorphone_HCl | Hydromorphone HCl | Yes |
| 0048T_10_1 | Methylphenidate_HCl | Methylphenidate HCl | Yes |
| 0048T_11_1 | Oxycodone_HCl | Oxycodone HCl | Yes |
| 0048T_12_1 | Cannabinol | Cannabinol | Yes |
| 0048T_13_1 | Methylphenidate_HCl | Methamphetamine HCl | Yes |
| 0048T_14_1 | Testosterone_acetate | Testosterone Acetate | Yes |
| 0048T_15_1 | TFMpp_HCl | Tfmpp HCl | Yes |
| 0048T_16_1 | AM2201 | AM2201 | Yes |
| 0048T_17_1 | HU-211 | HU-211 | Yes |
| 0048T_18_1 | JWH-251 | JWH-251 | Yes |
| 0048T_19_1 | 4-Butylone HCl | 4-Butylone HCl | Yes |
| 0048T_20_1 | 3-Fluoromethcathinone HCl | 3-fluoromethcathinone | Yes |
| 0048T_21_1 | 5-Methoxy_DALT | 5-Methoxy DALT | Yes |
| 0048T_22_1 | Levamisol_HCl | Levamisol HCl | Yes |
| 0048T_23_1 | Acetaminophen | Acetaminophen | Yes |
| 0048T_24_1 | D-(+)-Glucose | Dimethyl sulfone | No |
| 0048T_25_1 | Pentobarbital | Pentobarbital | Yes |
| | | **Accuracy** | **96%** |

### 3.5 Instrument to Instrument Reproducibility Results

Following the conformity testing of the primary MicroNIR, two additional MicroNIR spectrometers (serial numbers (S1-00129 and S1-00138) were also used to scan the illicit material conformity samples. Each instrument prediction results are found below in Tables 3 and 4.

Table 3: Prediction results for target MicroNIR serial number S1-00129.

| Unknown File ID | Predicted | Known ID | Match |
|---|---|---|---|
| 0129_01_1 | Methylone_HCl | Diltiazem HCl | X |
| 0129_02_1 | Inositol | Inositol | Y |
| 0129_03_1 | Niacinamide | Niacinamide | Y |
| 0129_04_1 | Procaine_HCl | Procaine HCl | Y |
| 0129_05_1 | Pseudoephedrine_base | Pseudoephedrine base | Y |
| 0129_06_1 | d,l-Amphetamine_sulfate | D,l-amphetamine sulfate | Y |
| 0129_07_1 | Carisoprodol | Carisoprodol | Y |
| 0129_08_1 | Cocaine_HCl | Cocaine HCl | Y |
| 0129_09_1 | Hydromorphone_HCl | Hydromorphone HCl | Y |
| 0129_10_1 | Naphyrone_HCl | Methylphenidate HCl | X |
| 0129_11_1 | Oxycodone_HCl | Oxycodone HCl | Y |
| 0129_12_1 | Cannabinol | Cannabinol | Y |
| 0129_13_1 | Naphyrone_HCl | Methamphetamine HCl | X |
| 0129_14_1 | Testosterone_acetate | Testosterone  Acetate | Y |
| 0129_15_1 | TFMpp_HCl | Tfmpp HCl | Y |
| 0129_16_1 | AM2201 | AM2201 | Y |
| 0129_17_1 | HU-211 | HU-211 | Y |
| 0129_18_1 | JWH-251 | JWH-251 | Y |
| 0129_19_1 | 4-Butylone HCl | Butylone HCl | Y |
| 0129_20_1 | 4-Fluoromethcathinone | 3-fluoromethcathinone | X |
| 0129_21_1 | 5-Methoxy_DALT | 5-Methoxy DALT | Y |
| 0129_22_1 | Levamisol_HCl | Levamisol HCl | Y |
| 0129_23_1 | Acetaminophen | Acetaminophen | Y |
| 0129_24_1 | Dimethyl_sulfone | Dimethyl sulfone | Y |
| 0129_25_1 | Pentobarbital | Pentobarbital | Y |
| | | **Accuracy** | **84%** |

Table 4: Prediction results for target MicroNIR serial number S1-00138.

| Unknown File ID | Predicted | Known ID | Match |
|---|---|---|---|
| 0138_01_1 | Methylone_HCl | Diltiazem HCl | N |
| 0138_02_1 | Inositol | Inositol | Y |
| 0138_03_1 | Niacinamide | Niacinamide | Y |
| 0138_04_1 | Procaine_HCl | Procaine HCl | Y |
| 0138_05__1 | Pseudoephedrine_base | Pseudoephedrine base | Y |
| 0138_06__1 | d,l-Amphetamine_sulfate | D,l-amphetamine sulfate | Y |
| 0138_07_1 | Carisoprodol | Carisoprodol | Y |
| 0138_08_1 | Cocaine_HCl | Cocaine HCl | Y |
| 0138_09_1 | Hydromorphone_HCl | Hydromorphone HCl | Y |
| 0138_10_1 | Naphyrone_HCl | Methylphenidate HCl | Y |
| 0138_11_1 | Oxycodone_HCl | Oxycodone HCl | Y |
| 0138_12_1 | Cannabinol | Cannabinol | Y |
| 0138_13_1 | Naphyrone_HCl | Methamphetamine HCl | N |
| 0138_14_1 | Testosterone_acetate | Testosterone  Acetate | Y |
| 0138_15_1 | TFMpp_HCl | Tfmpp HCl | Y |
| 0138_16_1 | AM2201 | AM2201 | Y |
| 0138_17_1 | HU-211 | HU-211 | Y |
| 0138_18_1 | JWH-251 | JWH-251 | Y |
| 0138_19_1 | 4-Butylone HCl | Butylone HCl | Y |
| 0138_20_1 | 4-Fluoromethcathinone | 3-fluoromethcathinone | N |
| 0138_21_1 | 5-Methoxy_DALT | 5-Methoxy DALT | Y |
| 0138_22_1 | Levamisol_HCl | Levamisol HCl | Y |
| 0138_23_1 | Acetaminophen | Acetaminophen | Y |
| 0138_24_1 | Dimethyl_sulfone | Dimethyl sulfone | Y |
| 0138_25_1 | Pentobarbital | Pentobarbital | Y |
| | | **Accuracy** | **88%** |

The instrument to instrument reproducibility results show promise implementing a direct calibration transfer to facilitate easy adoption of future new systems. The three spectrometers used in this trial included an early beta system and two early manufacturing build systems which were known to have distinct differences in manufacturing and is the cause for some of the misclassifications. This information was then utilized for creating instrument specification for us to target as a way to enable more successful method and library transfer from a master instrument to several other target instruments. Since this study was concluded at NFSTC, system-to-system reproducibility has been significantly improved as reported in a recent publication [4].

### 3.6 Mixtures & Detection level

In many cases, illicit substances are mixtures of pure components. In cases of illegal street drugs, the mixture consists of the active or controlled component (e.g. cocaine, heroin or amphetamine) and cutting agents (e.g. caffeine, paracetamol sucrose or lidocaine). Identification of these powder mixtures is challenging because of the wide variety of mixture components. Also, the active components and cutting agents found in street drugs vary with time and location. For example, new designer drugs are being introduced to the market every week. In Europe, cocaine is differently composed compared to the USA. Traditional quantitative or qualitative models are often based on a design of known constituents with pre-designed concentrations. Taking into account the practical issues of illicit substances, the construction of traditional models requires many samples and is therefore too costly and time consuming.

We therefore propose a calibration-free approach based on the concept of the net analyte signal (NAS) to identify powder mixtures [7]. This approach relies on expert knowledge about the main mixture components of a certain category of substances. In the first step, a certain category of illicit substances is defined, e.g. cocaine or heroin. Based on expert knowledge, these main categories are "filled" with so-called library components. These library components are pure substance components which can be found together as mixtures. Once a category is accurately documented with its library components, NIR spectra are collected for each library component. The subspace spanned by these library components is used for the identification model.

For an unknown sample, the NAS signal is calculated by projecting the unknown sample to the subspace spanned by the library components. The NAS for an unknown sample is the spectral response which is orthogonal to the spectra of the other library components. Next, the NAS vector is used to predict the composition of the unknown sample.

A set of library components were measured with MicroNIR serial number S1-2012-116. This specific MicroNIR unit is located in Amsterdam, The Netherlands. The library components are part of 4 illicit substance matrices: cocaine, heroin, XTC and amphetamine. These matrices were constructed based on the composition of street drugs commonly found in The Netherlands. From the matrices and its library components, an identification model was constructed dedicated to identify street drugs.

Next, a number of street drug samples were analyzed with MicroNIR S1-2012-116 by placing the sample directly on the window collar. The physical appearance of these street drug samples varies from fine powders to lumps or intact tablets. For law enforcement purposes, it is important to identify the controlled substance for a particular sample. Besides, the model also provides information about the existence of cutting agents. Like this, a more complete identification result can be accomplished. Such information is well suited for tactical information purposes e.g., to investigate if different samples originate from the same supplier.

Accordingly the identification model is used to predict the composition of the street drug samples. The street drugs identification model is constructed to minimize false positives. Furthermore, the detection limit of a component in a mixture is approximately 15 w/w% (depending on the complexity of the mixture). The identification results are presented in the second column of Table 4.

For each street drug sample, the composition was determined using GC-MS. The third column of Table 4 represents the outcomes of the GC-MS measurements. The weight percentage of each identified component is also listed. A weight percentage listed as (x) means the components weight percentage was < 5 w/w%.

From Table 4, it can be seen that the identification model is well capable in identifying controlled substances in multi-component mixtures.

Additionally, a total of 150 street drug samples were analyzed, resulting in 1.5% false negatives and 2% false positives. 28% of all samples contained controlled substances with weight percentages < 10 w/w%. These samples represented heroin samples containing small amounts of the controlled substance (heroine) and paracetamol + caffeine as cutting agents.

Table 4: Identification results for MicroNIR serial number S1-0116T.

| Unknown File ID | Predicted | Known ID (w/w%) |
|---|---|---|
| S1-0116T_1 | CocaineHCL \| Levamisol | Levamisol (15) \| Cocaine (70) |
| S1-0116T_2 | Caffeine \| CocaineHCL \| Phenacetine | Caffeine (5) \| Cocaine (44) \| Phenacetine (35) \| By-products (x) \|Lidocaine (x) |
| S1-0116T_3 | Caffeine \| HeroinBASE \| Paracetamol | Caffeine(24) \|Heroin (11) \| Paracetamol (x) \| Noscapine (x) \| Papaverine (x) \| 6-acetylcodeine (x) |
| S1-0116T_4 | Caffeine \| Paracetamol | Caff (33) \| Paracetamol (x) |
| S1-0116T_5 | Cellulose \|MDMAHCL \|Talcum | MDMA (29) |
| S1-0116T_6 | Amfetamine \| Caffeine \| Sucrose | Caff (78) \|Amf (6) \| Unknown (x) |
| S1-0116T_7 | Phenacetine | Phenacetine (94) |
| S1-0116T_8 | CocaineHCL \| Phenacetine. | Caffeine (1)\| Amfetamine (7)\| Levamisol (3) \|Cocaine (34) \| Phenacetine (24). |
| S1-0116T_9 | Cellulose \| Talcum | Caffeine (4) \|MDMA (5). |
| S1-0116T_10 | Caffeine \| Paracetamol. | Caffeine (30) \| Heroïn (6) \| Paracetamol (x) \| Noscapine (x) \| 6-acetylcodeine (x). |

The outcome of the identification model illustrates that the MicroNIR unit is able to provide enough distinctive spectral information for a wide range of illicit drug components. In the near future, the MicroNIR S1-2012-116 will be tested as a master instrument within a large field-test in the Netherlands. 15 other MicroNIR analyzers are being used in a cloud-computing environment by police officers to identify unknown mixtures in their daily routine work.

## 4. CONCLUSIONS

We have demonstrated that the MicroNIR spectrometer weighing < 60 grams (3 ounces) is able to identify controlled substances present in street drugs with a very low error rate of prediction. By combining innovations in miniature NIR spectroscopy and multivariate analysis, and leveraging the ever more ubiquitous smart devices and cloud computing, the MicroNIR spectrometer is a game changer for law enforcement agents, Interpol, and drug enforcement agents.

## 5. ACKNOWLEDGEMENTS

JDSU would like to thank Joan Ring and all other employees at NFSTC for their assistance with the data acquisition for this project.

## REFERENCES

[1] National Forensic Laboratory Information System (NFLIS) 2010 Annual Report, retrieved from: https://www.nflis.deadiversion.usdoj.gov/DesktopModules/ReportDownloads/Reports/NFLIS2010AR.pdf
[2] Macleod, H.A., [Thin-Film Optical Filters], Fourth Edition, CRC Press, Boca Raton, FL, 302-369, 490-513 (2010).
[3] O'Brien, N., Hulse, C., Friedrich, D., Van Milligen, F., von Gunten, M., Pfeifer, F., Siesler, H., "Miniature Near-Infrared (NIR) Spectrometer Engine For Handheld Applications." Proc. SPIE, Ed. M. Druy, and R. Crocombe, 8374, p 837404-1-8 (2012).
[4] Friedrich, D., Hulse, C., von Gunten, M., Williamson, E., Pederson, C., O'Brien, N., "Miniature near-infrared spectrometer for point-of-use chemical analysis." Proc. SPIE, Ed. Y. Soskind and G. Olson, 8992 (2014).
[5] Anderson, C.A., Drennen, J.K., Ciurczak, E.W., [Handbook of Near-Infrared Analysis], Burns, D. A and Ciurczak E. W. (editors), 3rd Edition, CRC Press, Boca Raton, USA, 585-611 (2008).

[6] C.-C. Chang and C.-J. Lin. LIBSVM : a library for support vector machines. ACM Transactions on Intelligent Systems and Technology, 2:27:1--27:27, 2011.

[7] Lorber, A., Faber, K.., Kowalski, B.R., "Net analyte signal calculation in multivariate calibration", Anal. Chem. (69), 1620-1626 (1997).