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Taking Presumptive Drug Testing from the Field to the Cloud!

For this issue I invited Dr. Richard Blair of the University of Central Florida (UCF) to expand on the presentation given by his graduate student, David Nash, at the 2014 National Institute of Justice Research and Development Grantees Meeting, which is held annually at the American Academy of Forensic Sciences meeting. The goal of Dr. Blair's research is to develop and commercialize a 3D-printed handheld spectrometer that can be used with a smartphone camera to acquire spectral data of suspected substances of abuse and then compare it to spectra in a cloud-based database. The approximate total material cost per custom-made spectrometer? $218. Compared to the tens of thousands of dollars spent by crime labs on color test field kits every year, this would provide a substantial cost benefit.

Dr. Blair joined the faculty at UCF in the winter of 2007 after receiving his Ph.D. in materials chemistry from UCLA. A few years later Dr. Blair's colleague, Kevin Andera at the Orange County Crime Lab, contacted him for help with a problem involving seized drug screening. Benzylpiperazine (BZP) was becoming popular as a party drug; however, the presumptive tests they had could not distinguish between BZP and MDMA, commonly known as ecstasy. The lab was forced to perform lengthy analysis with no way to prescreen, and Kevin asked Dr. Blair if he could find a solution to their problem. The observable fluorescence using d^{10} metal cluster compounds was very good across a range of substances, and they have been pushing the work forward since.

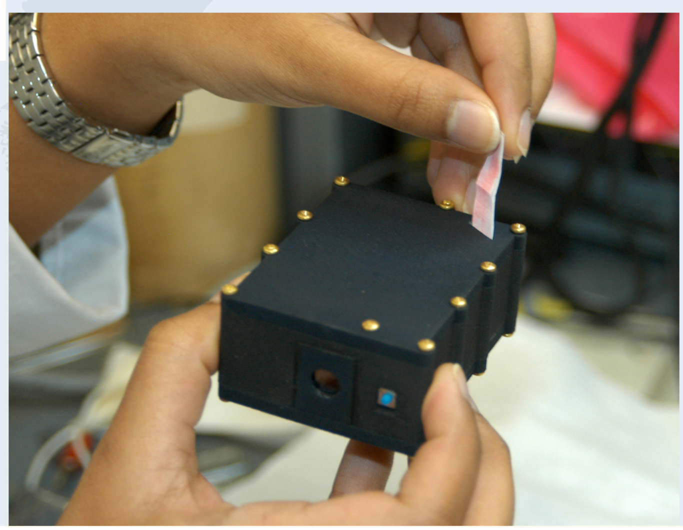
Ryan Tomcik: *What current methods are used for field detection of substances of abuse?*

Richard Blair: Current methods use a series of color tests. Examples of these tests are Marquis Reagent (concentrated sulfuric acid and formaldehyde) for identifying alkaloids and the Duquenois–Levine reagent (vanillin, acetaldehyde and ethanol) for identifying THC. The Narcopouch® facilitates safe implementation of these tests, but it does not eliminate the fundamental flaws in the tests. These methods often use toxic or dangerous reagents and destroy the analyte. Identification is dependant on accurate observations of the colors formed and their timing. Additionally, the origin of these colors is poorly understood. False positives can lead to highly publicized mistakes. Quite recently, a New York couple spent a month in jail when homemade soap gave a false positive for cocaine (See: *Drug suspects had soap, not cocaine bricks*, The Morning Call: Dec 2013).

What makes the d^{10} metal cluster compounds ideal for controlled substance testing applications?

Metal ions like Cu^{+}, Ag^{+}, Au^{+}, Cd^{2+}, and Zn^{2+} have a full set of d electrons even though their neutral forms do not. These ions can form molecular cubes with halogens like iodine to form a structure with the formula M_4X_4 where M is the metal and X is the halogen. When formed this cluster has a set of empty molecular orbitals that are close in energy to the lone pair of electrons in the nitrogen in an amine. A complex can form with the formula $M_4X_4L_4$. When illuminated with UV light, the metal-halogen cluster absorbs energy and can emit in the blue range. If the analyte forms molecular orbitals close enough in energy to the excited state of the metal cluster, then there can be energy transfer to these orbitals and subsequent emission in the visible. This is a well understood phenomenon firmly based in science and it has been studied for decades.

The color of the visible fluorescence is very sensitive to the structure of the analyte. This makes it ideal for controlled substance testing since minor variations in a compound's structure will produce visible differences in the observed fluorescence. Other advantages include low cost, specificity,



stability, non-destructiveness, adaptability, and objectivity with regard to user interpretation.

What classes of substances have you incorporated into your research so far?

We have screened a wide array of amines and common aldulterants. In addition, Wayne Moorehead at the Orange County (CA) Crime lab looked at barbital, benzocaine, benzylpiperazine, butabarbital, caffeine, "case work" cocaine, cocaine free-base "Rock," cocaine HCl, d-methamphetamine, MDMA, mescaline, PCP, pseudoephedrine, and trifluoromethylphenylpiperazine (TFMPP). Either no fluorescence or a unique color was observed for these compounds. Notably, this test is the only presumptive method that can distinguish between cocaine and PCP.

What effect does the presence of common cutting agents, such as flour or aspartame, have on your technique?

Cutting agents without amine groups will not form complexes with the d^{10} indicators and will not interefere with identification. Agents with amine groups (such as aspartame) may form complexes with the indicators, but the drug will as well. The result will be a spectra with two discernable peaks. We have not fully studied the spectra of mixtures. Work with case work cocaine suggests that adulterants or impurities will not adversely affect correct identification.

How did you conceive of the idea of a pocket spectrometer that can be used with a smartphone camera?

The idea for the spectrometer started out as a modified scanner for color identification. Initial work took a commercial scanner, removed the glass (which is not transparent to UV), and replaced the cold cathode light source with a UV cold cathode lamp. It worked, but color rendition was poor. We were going to do a lot of work in terms of calibration and accurate color identification. Then, I ran across an article in the magazine, *Chemical and Engineering News*, about open source software for reading cell phone, web cam, or any image data as spectra. I quickly realized that a device incorporating a diffraction grating would allow capture of true spectral data and eliminate interpretation. The ability to use a cell phone was an added bonus.

We use the cell phone's camera app to take a picture, and then we upload the image to the SpectralWorkbench website. The current implementation can use images from any source: webcam, iPad, laptop's camera. SpectralWorkbench is an opensource spectral analysis package: **www.spectralworkbench.org/**

The spectrometer body is produced using 3D printing. This allows us to rapidly assess designs and make changes without incurring large expenses.

How would an investigator use your device in a crime scene or field scenario?

An investigator would have a packet of test strips, pre-dipped in a saturated d^{10} salt solution and dried, a dropper of ethanol, and the spectrometer. The unknown would be rubbed or placed on the strip and a drop of ethanol would be added to facilitate mixing. Once dry, the strip can be quickly examined with an alternative light source and placed into the spectrometer. Then, a cell phone is pressed against the viewport and a photo is taken. In the future the photo will be analyzed using an app based on the SpectalWorkbench software.

Will crime scene investigators and law enforcement be able to use this technology in the near future?

The indicators are usable right now. They have a very low technology level and require minimal investment for usage. As is, they are probably more suited for screening in a crime lab. The cell phone spectrometer should be ready for rollout in a year, and we have already attracted the interest of a forensic supply company.

I am looking for testing volunteers. When we finalize the spectrometer design, we would like to produce multiple units for lab and field testing. The more users we have the better the identification database will get.

Where can people go, or who can they contact for more information on this project?

People can go to my group's website (**www.blair.research.cos.ucf.edu/#forensic**), or they can e-mail me directly at **Richard.Blair@ucf.edu**. If you are in Orlando and want to see the work, feel free to contact me to schedule a visit.

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