Y11 The Detection and Quantification of Trace Fentanyl in Mixtures With a Portable Raman Instrument and Chemometrics

Ling Wang, PhD, Florida International University, Miami, FL 33139; Mario O. Vendrell-Dones, BS, Florida International University, Miami, FL 33199; Sevde Dogruer, Bogazici University, Istanbul 34893, TURKEY; Bruce R. McCord, PhD, Florida International University, Miami, FL 33199*

Learning Overview: The goal of this presentation is to describe a detection method based on Surface-Enhanced Raman Spectroscopy (SERS) with a portable Raman instrument and a chemometric model to distinguish mixtures of fentanyl/heroin, fentanyl/cocaine, and fentanyl/heroin/cocaine.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by demonstrating a SERS-based chemometric method for the presumptive screening of opioids. This new method is fast and can rapidly distinguish fentanyl analogs from other drugs.

The abuse of opioids has become a critical issue in the United States over the past five years. New synthetic fentanyl analogs continue to appear in street drugs, resulting in increased threats to the public health. Since the appearance of these new fentanyls, prior screening methods, such as immunoassay, have had difficulty in the detection and analysis of the multiplicity of opioid analogs in the market. This study has been working on an alternative screening method using SERS coupled with metal nanoparticles and aggregating agents. SERS is a rapid screening method that provides molecular fingerprint signals at toxicological concentrations. The procedure is simple and fast, and it is convenient for use in both point-of-care analysis and laboratories. The new method can detect fentanyl analogs, cocaine, and heroin at low to sub ng/mL concentrations, as well as distinguish fentanyls in mixtures with cocaine or heroin, even at levels as low 0.01% fentanyl in the mixture.

The SERS method utilizes gold/silver nanostars in colloidal form that are mixed with magnesium chloride and aggregated. Next, drug samples are added to aggregated silver/gold nanostars and allowed to incubate for five minutes. On the surface of the aggregated nanostars, the creation of hot spots produces localized surface plasmon field effects resulting in an improvement in SERS enhancement. The SERS spectrum provides molecular vibration information that can identify individual compounds. Chemometrics, such as linear discriminant analysis and principle components analysis, were then used to create a model to cluster classes of drug samples, as well as distinguish single drugs and their mixtures. The resultant data assist in the calculation of the percentage of fentanyl in the mixture based on the composite spectra.

The SERS method permits a rapid, easily operated presumptive test for opioids. It is orthogonal to mass spectrometry and sufficiently sensitive to detect compounds at toxicological levels. As a result, it should be particularly useful for the screening of fentanyl analogs, mixtures with heroin and/or cocaine, as well as other novel psychoactive substances and mixtures.

Fentanyl Mixtures, SERS, Portable Raman

Copyright 2020 by the AAFS. Permission to reprint, publish, or otherwise reproduce such material in any form other than photocopying must be obtained by the AAFS.

*Presenting Author