B21 The Application of Surface-Enhanced Raman Spectroscopy (SERS) for the Detection of Opioids

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Learning Overview: The goal of this presentation is to describe the development and application of Surface Enhanced Raman Spectroscopy (SERS) for the presumptive determination of opioids and fentanyls. Information provided will include the optimized detection method, and the experimental and calculated spectrum.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by demonstrating the SERS method in the presumptive screening of opioids. The new method is fast and can rapidly distinguish opioids and fentanyl analogues.

Over the last five years, the abuse of opioids has been a critical issue to public health. The appearance of new synthetic fentanyls ever increase, the abuse of which threatens death; indeed, over 100 people in the United States die from overdose every day. Current screening methods, such as immunoassay, have difficulty detecting the full range of opioid analogues due to a wide variety of structural variations. This work shows an alternative screening method using Surface Enhanced Raman Spectroscopy (SERS) coupled with gold/silver nanostars and magnesium chloride aggregating agents. SERS is a rapid screening method that provides molecular fingerprint signals at toxicological concentrations. This work proves that this new method can distinguish fentanyl analogues and opiates at low to sub ng/mL concentrations. Additionally, this procedure is simple and fast to operate. The procedure is convenient for use in point-of-care analysis and in laboratory settings.

The SERS method utilizes the complex of gold/ silver nanostars and magnesium chloride. When the Au/Ag nanostars are mixed with magnesium chloride, these nanostars aggregate. Next drug samples are added to the aggregated nanostars and allowed to incubate 5 minutes. The solution is placed in a quartz well plate and analyzed via a Perkin Raman 400F instrument with laser excitation at 785 nm. Hot spots created between the aggregated nanostars results in localized surface plasmon field effects that produce a superior SERS enhancement. The SERS spectrum also provides a “fingerprint” that can be used to ascertain the chemical structure of target drug samples and identify individual compounds. Linear discriminant analysis and principle component analysis were also used to create a model to distinguish opioids based on the generated spectra. Additionally, in silico density functional theory modeling was applied to various fentanyl molecules and used to identify parameters necessary in calculating theoretical SERS spectra. The resultant data should prove useful in identifying unknown compounds and characterizing their interactions with the nanoparticle substrates. SERS technique has high sensitivity. Based on the aggregated nanostars method, the detectable limit of opioids can be 0.25 ng/mL to 25 ng/mL depending on the type of drug.

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 opioids and other novel psychoactive substances.

SERS, Opioids, Fentanyls