B19 The Development of a Rapid, Reliable Detection Method for Synthetic Cathinones

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Learning Overview: After attending this presentation, attendees will understand the principles of Surface-Enhanced Raman Spectroscopy (SERS), how the application of SERS is used to rapidly detect synthetic cathinones, and how selected bands can be utilized as markers of these substances.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by demonstrating the application of SERS to the detection of synthetic cathinones, such as 3,4-methylenedioxy-5-methylethcathinone and 4-methylethcathinone.

Effectively examining synthetic cathinones will contribute to the prevention of their proliferation and to the assistance of victims suffering from overdose, irreversible health damage, or even death. Improvements in the control of these compounds will also aid toxicologists and forensic scientists in detecting and limiting their effect on society. Furthermore, being able to detect these synthetic drugs will provide critical assistance in understanding the effects of these substances on the human body.

Currently, countless structural variations of new synthetic cathinones ("bath salts") appear in drug markets. However, the research into their specific toxicological effects in humans is lacking. Manufacturers synthesize these new synthetic cathinones in various ways, and many of these drugs are sold as mixtures containing additives. Variations in the purity of these drugs and, thus, the presence of additives at unknown concentrations, can cause overdoses. These mixtures cause problems for both policing and health agencies. Therefore, there is a need for a screening method that can assist authorities in identifying these drugs in a more rapid, sensitive, and inexpensive way.

Since the drugs studied in this proposal are structurally similar, SERS is uniquely suited as a screening procedure. Due to its molecular specificity and sensitivity, SERS constitutes an ideal platform to detect and differentiate synthetic cathinone analogs. SERS utilizes nanometallic surfaces to amplify the Raman signal of analytes, providing qualitative and quantitative information. The oscillations of the conduction electrons of these nanometallic structures causes the accumulation of photonic energy and results in Localized Surface Plasmon Resonances (LSPRs). LSPRs are responsible for the signal enhancement that allow adsorbed molecules to be detected, even at low concentration levels. LSPRs can also produce signal enhancements such that single molecule signals can be detected. This provides a flexible method to detect newly developed compounds and keep them off the streets.

The synthetic cathinones 3,4-methylenedioxy-5-methylethcathinone and 4-methylethcathinone have been analyzed with both traditional Raman spectroscopy and SERS. The methods for their detection have been optimized by varying pH, incubation time, nanoparticle size and composition, aggregating agents, and laser wavelength. Density Functional Theory (DFT) calculations have been used to assign the vibrational modes of major bands for each of the selected synthetic cathinones, providing a sound spectroscopic interpretation of the experimental Raman and SERS spectra. Further validation of this work will be completed with the ultimate aim of detecting these drugs and their analogs in biological matrices, starting with oral fluid.

Synthetic Cathinones, Surface-Enhanced Raman Spectroscopy, Density Functional Theory

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