K2 Surface-Enhanced Raman Spectroscopy (SERS) -Based Screening Test for Synthetic Cannabinoids in Oral Fluid

Irene Conticello, BS, University of Bologna, Dept of Chemistry "G. Ciamician," Via Selmi 2, Bologna 40126, ITALY; Chiara Deriu, MS, Florida International University, 11200 SW 8th Street, Miami, FL 33199; Thaddeus Mostowtt, MFS, 403 Lakeview Drive, Apt 101, Weston, FL 33326; and Bruce R. McCord, PhD, Florida International University, Dept of Chemistry, University Park, Miami, FL 33199*

After attending this presentation, attendees will better understand SERS and how it can be used to retrieve structural information from small molecules at very low concentrations. Attendees will also understand how this approach can be applied to the detection of xenobiotics in oral fluid.

This presentation will impact the forensic science community by demonstrating how SERS is a fast, selective, and sensitive approach for synthetic cannabinoids screening, as an alternative to immunoassays.

Synthetic cannabinoids are New Psychoactive Substances (NPS) that represent a worldwide issue due to unknown toxicological effects and widespread use among the young population. Moreover, the rapidity by which these compounds are modified and introduced into the illegal market makes it difficult to detect them using standard screening methods, such as immunoassays. Indeed, cross-reactivity between different species and false negative responses severely limit this approach.

SERS has been shown by this study to have great potential to solve these problems by providing a sensitive and selective screening approach that can provide fingerprint signals from xenobiotics at toxicological concentrations. This was achieved on benzodiazepines, both as standard solutions and in spiked urine matrices, and more recently, on standard solutions of synthetic cannabinoids. The latter included JWH-018, JWH-030, JWH-073, JWH-081, JWH-122, JWH-175, AM-2201, MAM-2201, with typical Limits of Detection (LODs) ranging from 20ng/mL for JWH-018 to 140ng/mL for JWH-081 and AM-2201. By translating this strategy to biological matrix analysis, the forensic and emergency medical field would benefit from a sensitive and selective alternative to current immunoassays. Because the procedure provides a spectral fingerprint, SERS can be seen as a complementary tool to other structure elucidation techniques, such as mass spectrometry.

SERS is a surface spectroscopy that amplifies Raman scattering by several orders of magnitude via the addition of metallic nanoparticles capable of producing Localized Surface Plasmon Resonance (LSPR). In this method, citrate-reduced gold nanospheres were prepared as LSPR-bearing substrates and later aggregated through the addition of $MgCl_2$. The aggregation process red-shifts the frequency of the LSPR and produces strong electromagnetic fields where the particles interact. The result is a rapid method for detection with exceptional sensitivity.

This presentation will focus on the development of an optimal extraction technique to detect synthetic cannabinoids in oral fluids. Fortified oral fluid samples were pretreated via centrifugation in the presence of methanol, which yielded protein sedimentation. Throughout the course of this work, thiocyanate anions were found to be a critical interfering species, as they strongly interact with the colloidal gold. Therefore, a variety of different desalting procedures were examined prior to SERS analysis, including ion exchange and solid phase extraction. The SERS signal was also increased through various wash steps conducted on the gold colloid, prior to its use as an enhancing substrate. This reduced residual citrate molecules carried over from the synthetic process, leaving the nanoparticle's surface more available for analyte adsorption.

The optimized methodology was developed using JWH-018 as a model target drug, then extended to other naphthoylindole synthetic cannabinoids. Detection was achieved using a portable Raman spectrometer operating at 785nm. This new procedure has great potential in forensic analysis, both as a more specific and flexible replacement for immunoassay and as an orthogonal method for analysis that is compatible with downstream mass spectral detection.

Major support for this research has been provided by an award from the National Institute of Justice. Points of view in the document are those of the authors and do not necessarily represent the official view of the United States Department of Justice.

SERS, Synthetic Cannabinoids, Oral Fluid

*Presenting Author