B15 Raman Spectroscopy and Multivariate Curve Resolution for Mixture Analysis of Forensic Drug Samples

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Learning Overview: The goal of this presentation is to describe the potential use of Raman spectroscopy coupled with Multivariate Curve Resolution (MCR) for analyzing multi-component samples commonly encountered in seized drug exhibits.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by demonstrating the utility of Raman spectroscopy for the analysis of complex mixtures that are difficult to effectively analyze by bulk spectroscopic analysis.

In recent years, there has been a rapid proliferation of new compounds emerging in the sphere of recreational drug use. These compounds are typically developed in an effort to stay ahead of drug scheduling laws banning their use and distribution. Keeping pace with the identification of these compounds is an increasing challenge for forensic labs. Most of these compounds are synthetically produced and are typically structurally similar to existing psychoactive substances. The compounds are constantly evolving and the lifecycles in the illicit drug market can vary. These factors make forensic drug analysis a moving target that points to the need for higher-throughput analytical methods that are also cost effective. The wave of Novel Psychoactive Substances (NPS) has resulted in a multitude of structurally similar compounds and closely related isomers that can be difficult to distinguish by some techniques. Differentiating these substances based on their vibrational spectra is generally straightforward for relatively pure materials. With complex mixtures or sufficient dilution, however, the utility of these techniques can be greatly diminished.

The objective of this work was to investigate the use of Raman spectroscopy for the identification of multiple constituents in mixtures. The method is intended to be a non-targeted screening approach with limited sample preparation requirements. By exploiting compositional variations in powder mixtures at the micro-scale, estimates of pure spectra of the constituents can be resolved using MCR techniques. The estimated pure spectra can be utilized more effectively in library searches, and detection limits can be significantly improved compared to mixture spectra from bulk spectroscopic analysis.

One motivation for this work was the detection of fentanyl and associated analogs in the presence of common cutting agents; however, the technique would be applicable to a broad range of drug classes. In evaluating this approach, this study utilized a surrogate for fentanyl, N-Phenethyl-4-Piperidinone (NPP), as a target compound. NPP is an intermediate in the synthesis of fentanyl that shares structural and spectral similarities. Raman data was collected using 830nm excitation on binary blends of NPP with 13 common cutting agents associated with fentanyl and heroin. In addition, NPP blends with multiple cutting agents as well as several over-the-counter medications that were also investigated. NPP levels down to 5% in blends were investigated in these studies and was readily identified in all samples using MCR. The results of these studies will be presented. This technique is currently being extended to seized drug materials to determine the effectiveness in real samples. Results of these investigations will also be presented, if available.

Raman Spectroscopy, Drug Analysis, Chemometrics

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