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## **Development of Validated Raman Spectral Libraries Using NIST Relative Intensity Correction Standards**

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Raman spectroscopy is a reagent-less analytical identification technique that is enjoying rapid growth because it can provide chemical sample identification in real-time and with a minimum of sample preparation. Because a useable Raman spectrum can be acquired through many types of packaging, a number of forensic laboratories are using the technique as a first-line analytical screening method for unknown compounds. Raman spectrometers are now being used at crime scenes, chemical spills, and other sites where remote or through-the-container analysis of an unknown may be important in protecting the safety of the investigative response team. Although the Raman method is not definitive, it can provide a rapid assessment of sample identity or sample class—often discerning the bad stuff from benign substances or in the case of pharmaceuticals, identify counterfeit from real product. Field deployable Raman instruments typically employ vendor-supplied Raman libraries. Comparing results between systems or within the same instrument under field conditions requires considerable expertise and experience on the part of the user and may not be possible if the spectrometer is not routinely calibrated. Our goal is to provide both the physical standards and the validated Raman spectral libraries necessary to impart confidence in these Raman measurements, to provide measurement traceability to national standards, and to ensure evidentiary acceptance of these measurements. This talk will discuss the generation of instrument-corrected Raman libraries, namely for Toxic Industrial Chemicals (TICs). The first step involves the qualification of the materials and the spectrometers used to generate the reference library. This process is modeled after the program to accept reference data into the OPCW (Organization for the Prevention of Chemical Warfare) database. This database and methods for accepting data were formed by an international treaty with nearly universal UN member state buy-in. The second step is the promulgation of this reference data and a new NIST/DHS supported website model will be discussed.

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