The Thermo Scientific Gemini Analyzer with LowDoseID for detection of low concentration illicit drugs

Introduction

The manufacture, distribution, and use of illicit drugs is a continuing and growing problem worldwide. The ability to detect and identify these types of substances in the field plays an important part in fighting this problem. One instrument that has been highly successful in detection and identification of illicit drugs is the Thermo Scientific™ Gemini™ Analyzer. The Gemini analyzer is the world's only handheld instrument that incorporates both Fourier transform infrared (FTIR) and Raman spectroscopies in one unit. These two spectroscopies are complimentary techniques and enhance the ability of a user to identify unknown substances in the field.

FTIR and Raman spectroscopy are excellent analytical techniques for identifying illicit drugs in pure form and in high concentrations in mixtures. However, in recent years the occurrence of low concentrations (1- 10 wt%) of illicit drugs such as fentanyl, fentanyl analogs, and heroin in powdered mixtures and pills has risen. Detection of these drugs in lower concentrations with standard FTIR and Raman spectroscopies can be challenging. To help local, state, and federal law enforcement agencies detect these lower drug concentrations in the field, we have has introduced the Gemini Analyzer with LowDoseID™. This instrument has two new enhancements:

1. The ability to use the SERS (surface enhanced Raman spectroscopy) based H-Kit.
2. The addition of a second Raman spectrum identification algorithm called Screener.

SERS based H-Kit

SERS is an analytical technique whereby molecules of a substance are first adsorbed onto the surfaces of nanostructures such as nanoparticles or roughened metal surfaces. The surfaces are typically gold and/or silver. These adsorbed molecules can then show an enhanced Raman scattering signal when illuminated with the laser used in a typical Raman spectrometer. This enhanced signal can be several orders of magnitude larger than a "normal" Raman signal, thus allowing for the detection of low concentrations of illicit drugs in mixtures and pills.

Our H-Kit consists of two parts. The first part is a plastic test stick which on one end contains a proprietary SERS substrate. The second part is a vial containing a solvent (either methanol or ethanol). To use this kit a user takes a small amount (typically 2 – 4 mg) of the substance of interest and places it in the solvent containing vial where it can dissolve. After dissolving as much of the substance as

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possible and letting any remaining solid material settle to the bottom of the vial, the SERS substrate is submerged into the solvent so that it is completely wetted. The SERS substrate is removed and then allowed to dry completely. To analyze the adsorbed chemical(s) the dry SERS substrate is placed into a specialized test stick adapter which has been previously attached to the end of the Gemini's Raman probe. A Raman spectrum is then acquired.

Screener algorithm

In addition to the standard Raman spectrum identification (ID) algorithm found on the Gemini, Gemini with LowDoseID now has a second Raman spectrum analysis algorithm called Screener. This algorithm is very similar to the one found in the Thermo Scientific™ TruNarc™ Analyzer; developed for identifying both pure drugs and drugs in mixtures. In contrast to the standard ID algorithm which answers the question "What unknown substances are present in my sample?" the Screener algorithm answers the question "Is a substance of interest present in my sample?". The Screener algorithm can analyze both normal Raman spectra and SERS H-Kit spectra.

The Screener algorithm uses an Alert Configuration file containing the substances that a user wants to screen for. The instrument comes with a preloaded default Alert Configuration file containing approximately 600 common illicit drugs, drug precursors, and cutting agents. These substances are placed into one of three classifications: Alarm, Warning, or Clear. The user can develop their own customized file by modifying this default file. Substances can be moved between the

classifications, added to the file from the instrument's 12,700 + item Raman factory library or from a user generated library, and deleted from the file.

Upon completing an analysis, the Screener algorithm will display the results in a hierarchical manner. If one or more Alarm items are identified, then only these will be displayed on the instrument's display screen. Even if substances in the Warning and Clear classifications are present and identified they will not be displayed. If no Alarm items are identified, then any identified Warning items will be displayed. Finally, Clear items will be displayed if no substances in the two higher classifications are identified. This contrasts with the standard ID algorithm which does not use the above classifications and will display all substances identified.

Illicit drug detection

The Gemini Analyzer with LowDoseID has over 700 illicit drugs, including fentanyl, heroin, cocaine, methamphetamine, fentanyl analogs, synthetic opioids, phenethylamines, synthetic cannabinoids, and cathinones, within its Raman factory library. It also contains numerous precursors, and many different cutting agents. Any of these items can be moved from the library to the Screener Alert Configuration file. The library also contains 40 SERS H-Kit spectra of common illicit drugs and cutting agents for use with the Screener algorithm. If an illicit substance is not present in the instrument's factory Raman library the software allows for a user to acquire their own library-quality spectrum and add it to a user library in the instrument.

Conclusion

The Gemini Analyzer with LowDoseID provides improved detection capabilities of illicit drugs with the addition of the SERS H-Kit and Screener algorithm enhancements. These new device capabilities provide low concentration detection of drugs in mixtures and pills. With low concentrations of very toxic drugs becoming increasingly common, the Gemini Analyzer with LowDoseID is a valuable addition to the analytical detection and identification toolbox of law enforcement and border protection.

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