

# Identification of Illicit Drugs and Hazardous Compounds with the Agilent 4500a FTIR Spectrometer

## Application Note

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### Introduction

FTIR spectroscopy is a proven, powerful technology for the analysis of illegal substances and potentially hazardous compounds. This results from the ability to rapidly measure the molecular fingerprint of a substance and compare it to libraries of known compounds. Thus, the identity of an unknown liquid or solid substance can be determined in less than 1 minute, with little or no sample preparation required.



*Figure 1. Agilent 4500a Series FTIR Portable Spectrometer equipped with diamond ATR sample interface. The system is battery powered, weighs less than 15 lbs and is fully portable.*

On-site analysis by portable FTIR systems is particularly useful since it can be used to establish probable cause, allowing for the seizure of materials for further analysis. It can also reduce the audit trail and shorten the chain of evidence, minimizing the potential for a compromised investigation. Some mobile FTIR spectrometers are designed for the most challenging environments such as hot zones, but these spectrometers tend to be expensive since they must be waterproof and impervious to liquid bleach required for decontamination procedures. The Agilent 4500a FTIR Spectrometer is a better, more cost efficient solution for the analysis of counterfeit drugs, illicit drugs, and hazardous substances (Figure 1). In this application note, the Agilent 4500a FTIR spectrometer equipped with diamond ATR sample interface is used to rapidly identify a series of illicit drugs.

Personnel involved in border control, corporate safety, mail room and post office security, as well as counterfeit pharmaceuticals and narcotics interdiction, will find the 4500a FTIR portable spectrometer a powerful aid in their important efforts to identify white powders, unknown chemicals, explosives, and illegal drugs.



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## Fast, accurate analysis of unknown substances

The 4500a FTIR spectrometer enables law enforcement officials to rapidly identify chemical substances on-scene. This powerful, fully portable system measures and identifies unknown solids, pastes, gels, and liquid chemical substances.

4500a FTIR portable spectrometer advantages include:

### Versatility

- Full portability for on-scene investigation or for deployment in mobile field labs
- Rapid screening and immediate answers to provide a better representation of the magnitude of the scene and enable personnel to make actionable decisions

### Ease-of-use

- All operation and analysis functions are controlled through a handheld PDA with a simplified user interface that handles data acquisition, analysis, and result reporting. One-button analysis is provided through pre-stored methods.
- Diamond ATR sample interface simplifies the analysis of solids and liquids while ensuring the sensor is protected against chemicals and physical abrasion.
- Liquid and solid unknown samples are measured in less than 1 minute without any sample preparation required.

### Performance

- Analyzer optomechanical components and electronics are engineered for class leading performance and ruggedness, ensuring reliable operation and trustworthy results.
- Uses Fourier transform infrared spectroscopy, which is well established within the forensic field
- Powerful search algorithm combined with extensive on-board database of hazardous substances and illegal drugs ensures fast accurate answers
- Unknown substance identity and quality of match to known substance contained in database is clearly displayed.
- Agilent Forensic Library contains the spectra of more than 13,000 biochemicals, white powders, HPV chemicals, toxic chemicals, food additives, and explosives.

## Instrumentation, materials, and methods

Samples of common illicit street drugs including cocaine hydrochloride, cocaine base, diacetylmorphine, morphine hydrochloride, and ketamine were measured using an Agilent FTIR spectrometer equipped with single reflection diamond ATR sample interface. Spectra were collected at

4  $\text{cm}^{-1}$  resolution with a total measurement time of less than a minute. The search algorithm employed was a simple similarity index measurement for ease of matching.

The sample consisted of approximately 5 mg of solid, which was placed on the diamond ATR sensor. The ATR solids press was used to ensure proper contact between the sample and the diamond ATR sensor. The Agilent Forensic Library was used for determining the identity of the unknown powders. Cleanup after measurement consisted of wiping the sensor with a small amount of acetone to remove the compound and any remaining traces. All data are date and time logged automatically.

## Results and Discussion

The five samples of illegal drugs were measured and then searched against the spectra of reference compounds contained within the Agilent Forensic Library. This analysis was carried out using MicroLab Mobile Software with a handheld computer, and yielded excellent identifying matches (for example, Figure 2). Subsequent analyses using a laptop computer equipped with Agilent MicroLab Software are also displayed (Figure 3). In the latter case, the fully automated search function displays the spectrum of the unknown sample, the spectrum of the best library match, the identity of the unknown, and a quantitative measurement of the quality of the match.

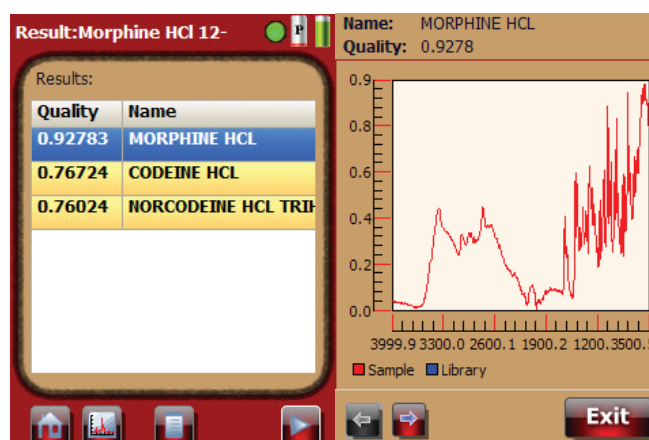


Figure 2. After spectra of an unknown is acquired, a preloaded method automatically searches an on-board forensic substance library and displays both the identity of the unknown, the quality of the match as well as the spectrum of the material on the PDA.

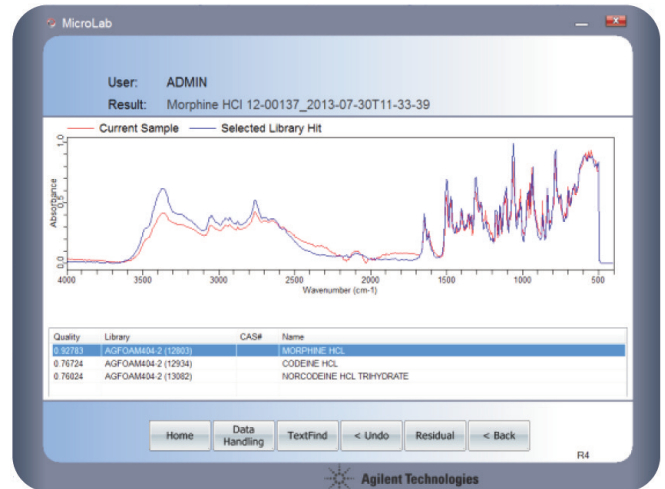
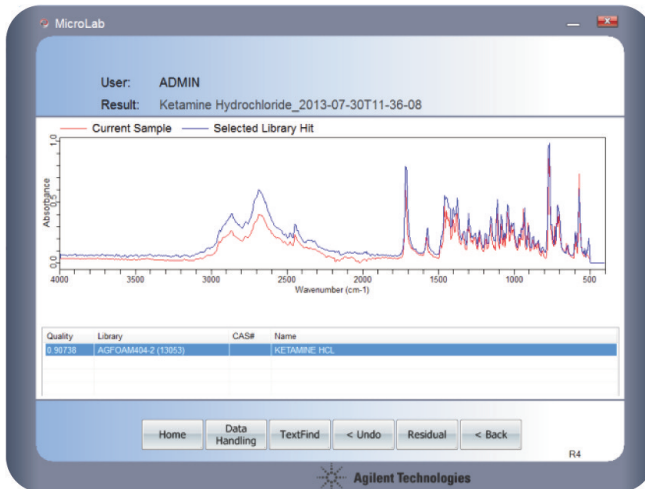
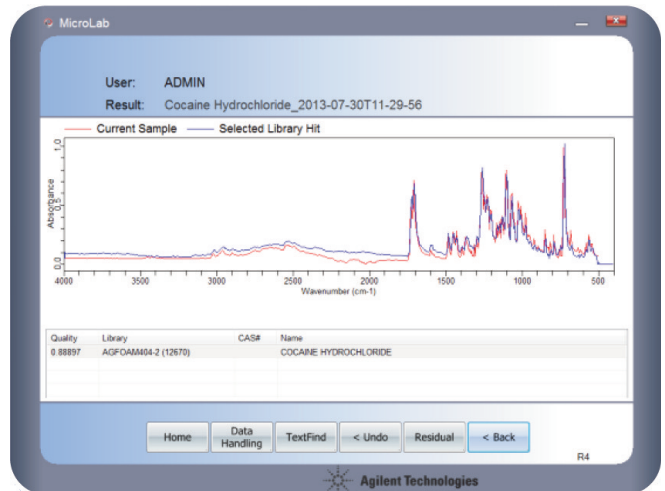
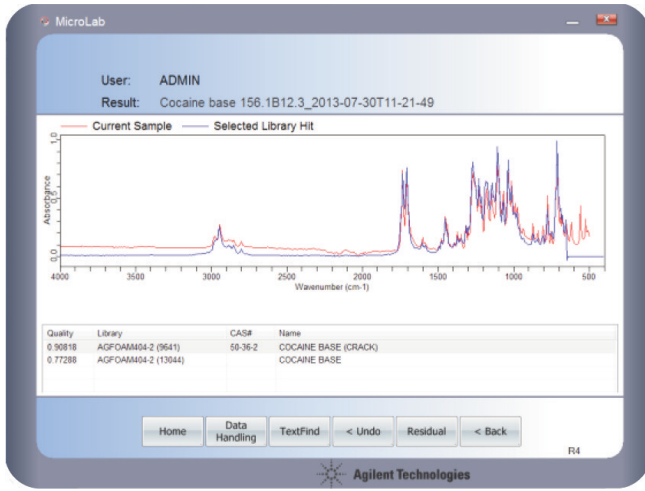


Figure 3. The Agilent 4500a FTIR spectrometer can be connected to a laptop computer for additional analyses of spectra. In this case, the spectra of a variety of unknown street drugs were searched against the Agilent Forensic Library, yielding excellent results. In addition to presenting the identity of the substance, the spectrum of the unknown sample and that of the best matching spectrum retrieved from the on-board library are displayed along with a numerical quality of the match.

## Conclusion

Personnel involved in detecting and identifying illegal contraband including illicit street drugs, counterfeit pharmaceuticals, as well as analyzing unknown chemicals and explosives, require measurement devices that provide them with on-scene answers. The Agilent 4500a FTIR, a portable battery powered infrared spectrometer, is an accurate, cost effective means of rapidly ascertaining this information. This enables actionable decisions to be made on-the-spot with respect to evidence gathering, and helps to reduce the likelihood of a compromised investigation.

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