



Application Note AN M117 Analysis of laced Drugs

The legal and illegal drugs comprise a wide range of different substances that differ strongly in their chemical and pharmacological characteristics. The number of available drugs in the market is constantly growing as new drugs are systematically synthesized with the intent to bypass the current narcotics laws. Most street drugs are not pure substances but mixtures that consist of two or more components. In order to maximize profits or to widen the spectrum of activity, drugs are laced with all kinds of substances or cut with other drugs.

As cutting agents usually substances are used that have chemical and physical properties similar to the drug itself. This prevents the detection of the contamination when the drug is for example solved or melted. The local anesthetic cocaine is being cut with other local anesthetics such as lidocaine or benzocaine in order to pretend higher cocaine content. Other often used cutting agents are milk sugar, pain relievers such as paracetamol, caffeine and the antiparasitic agent levamisole that is normally used in veterinary medicine. Many drug deaths are directly linked to these cutting agents. Many serious side effects, including deaths, were reported from cocaine contaminated with levamisole. In practice it is often important to rapidly analyze such substance mixtures in order to supply medical aid or to expose criminal acts like the sale or smuggling of drugs.

Keywords	Instrumentation and Software
FT-IR	ALPHA II Drug Identifier
Laced drugs	OPUS TOUCH Software
Mixture analysis	TICTAC ATR-FT-IR Drug Library
Identification	ATR-FT-IR-library for Forensics
Legal highs	IP65 certified touch-PC



Figure 1: ALPHA II Drug Identifier with touch-PC (right). Samples are directly pressed onto the ATR crystal for analysis (left).

The ALPHA II Drug Identifier is an ideal tool for the identification of pure and laced drugs. The analysis is based on infrared spectroscopy which is also called molecular spectroscopy. Infrared light induces vibrations of the molecules in the analyzed sample. The IR-light is therefore, depending on the sample characteristics, partly absorbed by the sample at specific wavelengths. The position and the intensity of the measured absorption peaks can be used for the identification of samples and mixtures. With the ALPHA II, the measurement of the spectra is performed by using the Attenuated Total Reflection (ATR) technique. Thereby the sample needs to be simply pressed on a diamond crystal by using a pressure clamp. Apart from the homogenization of the sample there is no need for sample preparation, also no consumables or chemicals are required. Identification of the respective drug sample is being performed by an automatic search of the measured spectrum in spectral libraries.

Standard Search



Figure 1: Spectra search of mephedrone. Red = measured spectrum, blue = library spectrum.

In the drug analyses shown in this application note, the spectrum search was performed by using the TICTAClibrary that contains over 500 spectra of newest drugs and "legal highs" and the ATR-FT-IR-library for Forensics that contains over 10.000 spectra of a wide variety of substance classes. In combination with these libraries the ALPHA II FT-IR spectrometer is able to detect pure substances as well as mixtures of drugs. The standard search algorithm of the OPUS software is very powerful in finding the library spectrum matching best with the measured spectrum. Though, in cases of mixtures the measured spectrum might contain spectral contributions from several library spectra. To determine the different components present in such mixture spectra, OPUS offers a specialized algorithm for the analysis of mixtures. The mixture analysis determines within only a few seconds and fully automated the composition of a mixture.

Example: The analysis of a pure drug.

The drug mephedrone is a former "legal high" and is forbidden in the EU since 2010. The spectrum shown in figure 1 was measured on a Platinum ATR-unit equipped ALPHA II FT-IR spectrometer with diamond crystal ("ALPHA II-P"). The spectra libraries were searched for a matching reference spectrum using the OPUS standard algorithm. When considering the very high similarity of the sample- and library-spectrum as well as the very high hit quality of 967 out of 1000 points it is obvious that the sample is most likely a pure substance. This is of course, as shown above, an exception since street drugs are very often contaminated as we are going to demonstrate in the next two examples.

Example:

Analysis of laced cocaine-hydrochloride

This example shows the analysis of cut cocainehydrochloride. Therefore a sample was measured with an ALPHA II-P spectrometer and a measurement time of 25



Figure 2: Mixture-analysis of laced cocaine-hydrochloride (red = measured spectrum, violet = composite, green = residual).

seconds. The result of the mixture analysis is shown in figure 2. For the sake of clarity only the measured spectrum (red), the composite spectrum (calculated from the found single components, violet) and the residual spectrum (green) are shown. The residual spectrum shows the differences between the calculated composite spectrum and the measured spectrum. The more even and flat the residual spectrum is, the better the match between the calculated composite spectrum and the measured spectrum. In our example we have a nearly perfect match between the composite spectrum and the measured spectrum, thus the peaks of the residual spectrum are of only limited intensity. Besides the main component cocaine-HCI the local anesthetikum anaesthesin (benzocaine) was found. The given percentage points describe the spectral contribution of the single components to the overall spectrum. Figure 3 shows the measured and the composite spectrum together with the spectra of the single components in detail.



Figure 3: From top: Measured spectrum, composite spectrum, component benzocaine, component cocaine HCl.

Example:

Analysis of "crack".

Crack is being made from cocaine salt (usually cocainehydrochloride) by heating it together with sodium bicarbonate (baking soda). Thereby, amongst others, the free cocaine base is formed. In contrast to cocainehydrochloride it can be smoked because of its lower melting point. Crack is usually laced too and is only rarely available as a pure product. Figure 4 shows the mixture analysis of a real street sample that was also measured with the ALPHA II-P. It is obvious from the mixture analysis



Figure 4: Mixture-analysis of laced crack (red = measured spectrum, violet = composite, green = residual).

result, that the sample is also laced with the local anesthetic anaesthesin. Additionally there is also a considerable amount of the pain reliever acetophenetidine (phenacetin) detectable. Acetophenetidine acts as a mild mood enhancer and is, due to its renal toxicity, forbidden in most countries. Due to its similar physical properties it is, however a widely used cutting agent and is used sometimes in very high concentrations.

Summary

The ALPHA II Drug Identifier with its simple touch operated user interface allows analyzing drugs and drug mixtures in a fast and comfortable manner. The combination of the dedicated drug library TICTAC and the very broad ranging "ATR-Forensics"-library identifies drugs, legal highs, unusual cutting agents as well as such substances that only appear to be a drug.

Bruker Scientific LLC

Billerica, MA · USA Phone +1 (978) 439-9899 info.bopt.us@bruker.com

Bruker Optics GmbH & Co. KG

Ettlingen · Germany Phone +49 (7243) 504-2000 info.bopt.de@bruker.com

Bruker Shanghai Ltd.

Shanghai · China Tel.: +86 21 51720-890 info.bopt.cn@bruker.com

www.bruker.com/optics

Bruker Optics is continually improving its products and reserves the right to change specifications without notice. © 2021 Bruker Optics BOPT-01