Realtime Detection and Fingerprint Analysis of Illicit Drugs

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Forensic chemical analysis aims to determine if a substance confiscated by legal forces contains an illegal compound, and if so, its purity and preferably origin. Confirmatory tests that unambiguously identify the potential drug and related impurities provide necessary evidence for law enforcement and for the courts to pursue criminal charges and to determine sentencing. Many drugs contain specific impurities from the manufacturing process, or compounds that are intentionally added in order to enhance or modify the drug effect. Their identification is a clue that helps law enforcement to identify sources of raw ingredients and track the distributors.

Fast and Sensitive Detection of Trace Cocaine Vapor

The TOFWERK Vocus TOF mass spectrometer directly and nondestructively analyzes samples in a real time. Further, the measurement doesn't require any sample preparation. An example of a Vocus measurement is shown in Figure 1. A local Department of Police and Customs provided small amounts of confiscated cocaine

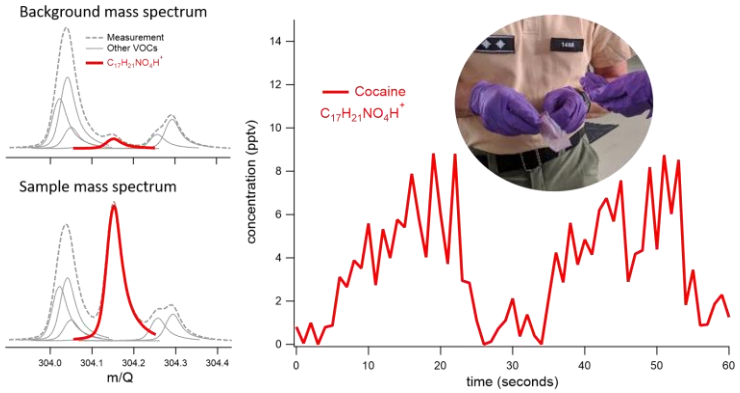

Figure 1 Vocus TOF analysis of confiscated cocaine. *A small bag containing cocaine was opened several times in front of the instrument inlet. Enhancement of the cocaine molecule at ppt levels is observed. The high resolving power of the instrument (Vocus S, dm/m=6000) allows the unambiguous measurement and identification of the peak at m/Q 304 $C_{17}H_{21}NO_4{\cdot}H^+$.*

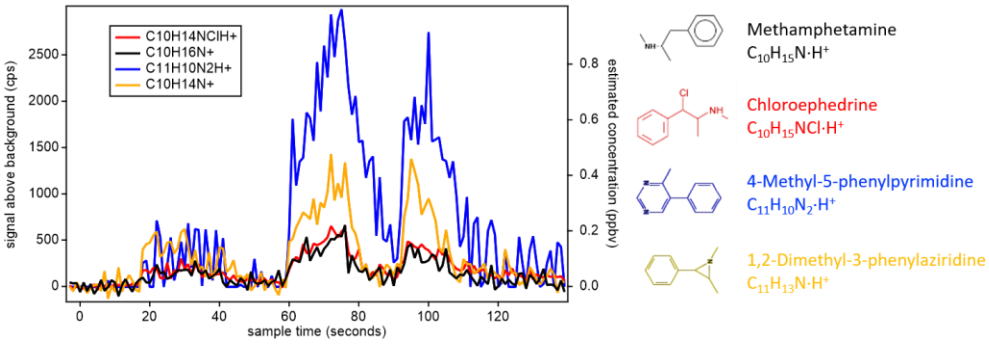

Figure 2 Forensic analysis of methamphetamine. *A bag containing a small amount of confiscated methamphetamine ($C_{10}H_{15}N$) was opened three times in front of the Vocus sampling inlet. The panel on the left shows the detected concentration of methamphetamine (black) and other vapors as the bag is opened. The elemental composition of these vapors is provided by the high resolving power, and the chemical identities on the right were determined by a comparison with known impurities described in scientific literature.*

sealed inside a plastic bag. The bag was simply opened and held in front of the instrument inlet for a few seconds. Although this analysis was conducted in a chemically complex, non-laboratory environment (a garage with high concentrations of gasoline and other fumes), the cocaine molecule (detected as $C_{17}H_{21}NO_3{\cdot}H^+$) is clearly visible as sharp enhancements above background that correspond with pulses of vapor from the bag. The high resolving power of the instrument enables the clear separation of the cocaine molecule from the many other VOCs present in the garage.

Fingerprint Analysis of Methamphetamine

The response of the Vocus TOF to any molecule is generally predictable, therefore no database is needed to make a first-order assessment of whether certain drugs are present. Illicit drugs are however chemically complex mixtures containing substances in addition to the active ingredient. More than 90% of a confiscated sample can consist of filler material, leftover contaminants from the synthesis, or specific adulterants. These compounds are often volatile and present in higher amounts than the drug itself, therefore they can be easily detected by the Vocus TOF directly in the gas phase and a chemical fingerprint unique to each drug sample can be obtained. These fingerprints differ based on the synthesis method, drug purity, storage and handling. Comparison of the detected impurities to a database or to impurities published in scientific literature can provide additional information.

For instance, the synthetic origin of methamphetamine can be suggested by examining the impurities. Illicit methamphetamine is typically made via one of six chemical recipes, each of which has characteristic byproducts[1]. Figure 2 shows the Vocus measurement of confiscated methamphetamine. In addition to the methamphetamine molecule itself, other substances identified as known byproducts of methamphetamine production were detected. In this sample, the

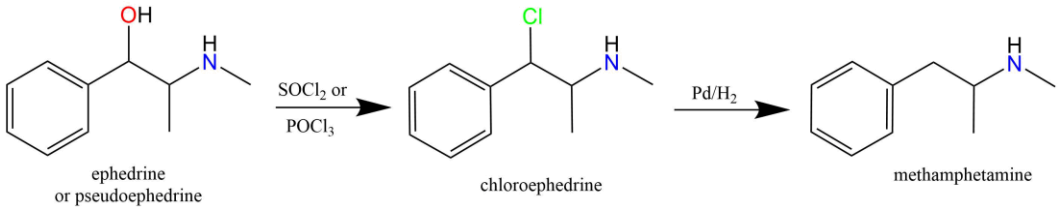

Figure 3 Emde synthetic pathway. *The presence of 1,2-dimethyl-3-phenylaziridine and chloroephedrine in the sample are indicative markers of the Emde synthetic method.*

impurities were more abundant than methamphetamine itself!

Because the whole mass spectrum is measured simultaneously, isotope patterns can be used to confirm the elemental composition of the detected substances, especially for unusual molecules such as cholorephedrine ($C_{10}H_{15}NCl$). The presence of 1,2-dimethyl-3-phenylaziridine and chloroephedrine are indicative markers of the Emde synthetic method[2] (Figure 3).

References

1. Des and Ismail, Impurity Profiling of Amphetamine and Methamphetamine Using Gas Chromatography Mass Spectrometry (GCMS) Harmonised Methods, Sains Malaysiana, 46 (1), 149-156, 2017.
2. Ko et al., The impurity characteristics of methamphetamine synthesized by Emde and Nagai method, Forensic Science International, 170 (2-3), 142-147, 2007.

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