New process for screening old urine samples reveals previously undetected 'designer drugs'

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Researchers from the University of B.C. and the BC Provincial Toxicology Center (BCPTC) have developed a more efficient way to

find out which new 'designer drugs' are circulating in the community.

In a study published in *Analytical Chemistry*, they showed how high-resolution mass spectrometry can be used to analyze urine samples at scale and uncover molecules from emerging designer drugs that have been missed by conventional testing.

The approach can support public health and safety by enabling swift identification of new substances, potentially saving lives and guiding timely clinical responses to drug-related emergencies.

"We were able to detect a number of drugs circulating in B.C. that were not being detected by existing tests. Any time such drugs emerge locally, that's important information for clinicians and public health officials to have," said Dr. Michael Skinnider, the study's lead author who conducted the research as an MD/Ph.D. student at UBC and is now an assistant professor at Princeton University.

Designer drugs have proliferated in the past two decades in the unregulated market. They tend to be modified versions of other drugs, with similar effects but just enough structural changes to get around drug laws. The drugs do not undergo proper testing or regulation. Some can poison or even kill users.

The BCPTC at the BC Center for Disease Control (BCCDC) has identified over 20 different drugs of concern while monitoring for them since 2020.

To confirm whether a drug is present in a sample, a lab must first know what they're looking for and obtain that drug in synthetic form. This becomes their "reference standard," and it's used to develop a repeatable laboratory test that leaves no doubt about the substance's presence.

However, reference standards can be hard to acquire. Sometimes the drugs are so new that a reference standard simply doesn't exist. Sourcing hundreds of reference standards for drugs that may or may not show up in the community is expensive and impractical, so laboratories instead make educated guesses about which ones to acquire.

The goal of the UBC/BCPTC study was to find a better way to prioritize acquisition of reference standards.

To do this, the researchers used high-resolution mass spectrometry to re-analyze more than 12,000 urine samples collected in B.C. from 2019 to 2022. If you imagine a urine sample to be a jigsaw puzzle with all its pieces scattered in the form of molecules, mass spectrometry can precisely determine the weight and shape of each puzzle piece, which helps researchers figure out which ones fit together in combinations that are typical of illicit drugs.

If a laboratory anywhere in the world has published data about new drug molecules found in their samples, a lab in B.C. can compare its data with theirs and determine which drugs are most likely showing up locally.

It's not a definitive confirmation, but it's enough to point the lab toward the right reference standards for more thorough testing.

The retrospective analysis of B.C. samples at BCPTC surfaced new synthetic opioids, benzodiazepines and stimulants that had eluded identification during initial screening. One of them, fluorofentanyl, is a modified version of fentanyl that was absent from samples before mid-2022 and then spiked during the final few months of the study. This suggests it was introduced to the local drug supply quite suddenly.

A few of the other drugs also had distinct peaks during the two-year study period.

"Applying this process on a regular basis will allow us to respond much more quickly to the emergence of new drugs and greatly reduce the time between a drug's introduction to the community, and our ability to test for it in a rigorous way," said Dr. Aaron Shapiro, the study's senior author who is a clinical assistant professor in UBC's department of pathology and laboratory medicine, and associate scientific director of the PTC.

The BCCDC is in the process of implementing this new tool into its clinical urine drug screen and hopes to apply it to other datasets in the future.

Researchers from the chief medical examiner's office in San Francisco and St. Paul's Hospital in Vancouver also contributed to the study.

More information: Identification of emerging novel psychoactive substances by retrospective analysis of population-scale mass spectrometry datasets, *Analytical Chemistry* (2023). DOI: 10.1021/acs.analchem.3c03451

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