

# Data-sharing website may speed the response to new illegal drugs

July 5 2018



The NPS DataHub allows forensic chemists to share data on new drug analogs, including their chemical structures and signatures, which are the keys to identifying them in the lab. Identifying drugs quickly is critical. "If people start overdosing and dying from a new drug analog, authorities need to identify it as quickly as possible," said NIST research chemist Aaron Urbas. "To focus your resources effectively, you need to know what you're looking for." Credit: German Federal Police (BKA)

The drug overdose epidemic currently gripping the nation is so tenacious in part because it's being driven by fentanyl, a synthetic opioid that comes in many forms. Each form has a slightly different chemical

structure, and clandestine chemists are constantly cooking up new ones. From a law-enforcement perspective, this makes fentanyl a moving target and very difficult to control.

To help with this situation, scientists at the National Institute of Standards and Technology (NIST), the German Federal Criminal Police Office (the Bundeskriminalamt, or BKA) and the U.S. Drug Enforcement Agency have launched a website where forensic chemists can share data on new drug variants, also called drug analogs. Described in *Forensic Chemistry*, the NPS Data Hub (NPS stands for Novel Psychoactive Substances) includes the chemical structures of drug analogs and their chemical signatures, which are the keys to identifying them in the lab.

Being able to identify drugs quickly is critical. "If people start overdosing and dying from a new drug [analog](#), authorities need to identify it as quickly as possible," said Aaron Urbas, the NIST research [chemist](#) who led the project. "If you want to focus your resources effectively, you need to know what you're looking for."

The goal of the NPS Data Hub is to get drug identification data to forensic chemists more quickly. In addition to data on synthetic opioids such as fentanyl, the Data Hub is also intended to cover synthetic cannabinoids (aka synthetic marijuana), synthetic cathinones (aka bath salts), amphetamines and other dangerous drugs.

## **New analogs can be hard to identify**

Underground chemists create new analogs in part to boost drug potency, with some fentanyl analogs being thousands of times stronger than heroin. This increases the risk to users, who may not know exactly what they're consuming. New analogs also allow the manufacturers to stay one step ahead of the law.

When drug evidence is seized, forensic chemists will often try to identify it using an instrument such as a mass spectrometer, which generates a unique barcode-like pattern—a sort of chemical signature—for the compound in question. They will then search law enforcement databases for a known compound with the same signature.

If the drug is new, the signature won't be recognized, and a much more complex analysis will be needed to identify the substance and determine its chemical structure. Few labs have that capability, so the drug may need to be sent to a more advanced facility. The whole process can take six months or more, including quality control to ensure the accuracy of the chemical structure and other data.

After that process is complete, the new drug and its chemical signature are added to law enforcement databases so that it can be identified more easily next time around."

We want to shorten the time lag between discovery of a new drug and the distribution of the data needed to identify it," Urbas said.

## **A different approach**

The NPS Data Hub aims to shorten that time lag by making it easier for experts to collaborate. For instance, a chemist from one lab can analyze a new drug and upload a proposed [chemical structure](#) and supporting data to the Data Hub. Then a second chemist from a different lab can review the data and confirm the proposed structure or suggest a new one.

"These people have very rare expertise," said NIST senior policy advisor Jayne Morrow. "The Data Hub brings these experts together and provides a forum where they can discuss what they're seeing in real time. There haven't been great ways to do that before, and it's really needed."

Only labs with sufficient capabilities can propose and confirm chemical structures. But other labs, including smaller state and local labs, can use that data.

In addition to the collaboration mechanism, the NPS Data Hub differs from existing drug databases in two ways. First, many databases only include [chemical](#) signatures based on commonly used techniques such as mass spectrometry. The NPS Data Hub permits sharing of analytical data from any technique, including Nuclear Magnetic Resonance (NMR), Raman spectroscopy, and others that, though less common, can be useful for differentiating closely related compounds.

Second, in commonly used drug databases such as the one maintained by the Scientific Working Group for the Analysis of Seized Drugs ([SWGDRUG](#)), the information is highly vetted for quality control. That makes SWGDRUG data authoritative, but the vetting takes months to complete. The [NPS Data Hub](#) is meant to be less authoritative but updated more frequently.

"The Data Hub can contain both curated and preliminary data, so you wouldn't necessarily use it to produce courtroom evidence," Urbas said. "But for tracking the emergence of new [drug](#) analogs, even preliminary data can make a huge difference."

**More information:** Aaron Urbas et al, NPS Data Hub: A web-based community driven analytical data repository for new psychoactive substances, *Forensic Chemistry* (2018). [DOI: 10.1016/j.forc.2018.05.003](https://doi.org/10.1016/j.forc.2018.05.003)

Provided by National Institute of Standards and Technology

Citation: Data-sharing website may speed the response to new illegal drugs (2018, July 5)

retrieved 30 June 2024 from <https://phys.org/news/2018-07-data-sharing-website-response-illegal-drugs.html>

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