Researchers develop AI to detect fentanyl and derivatives remotely

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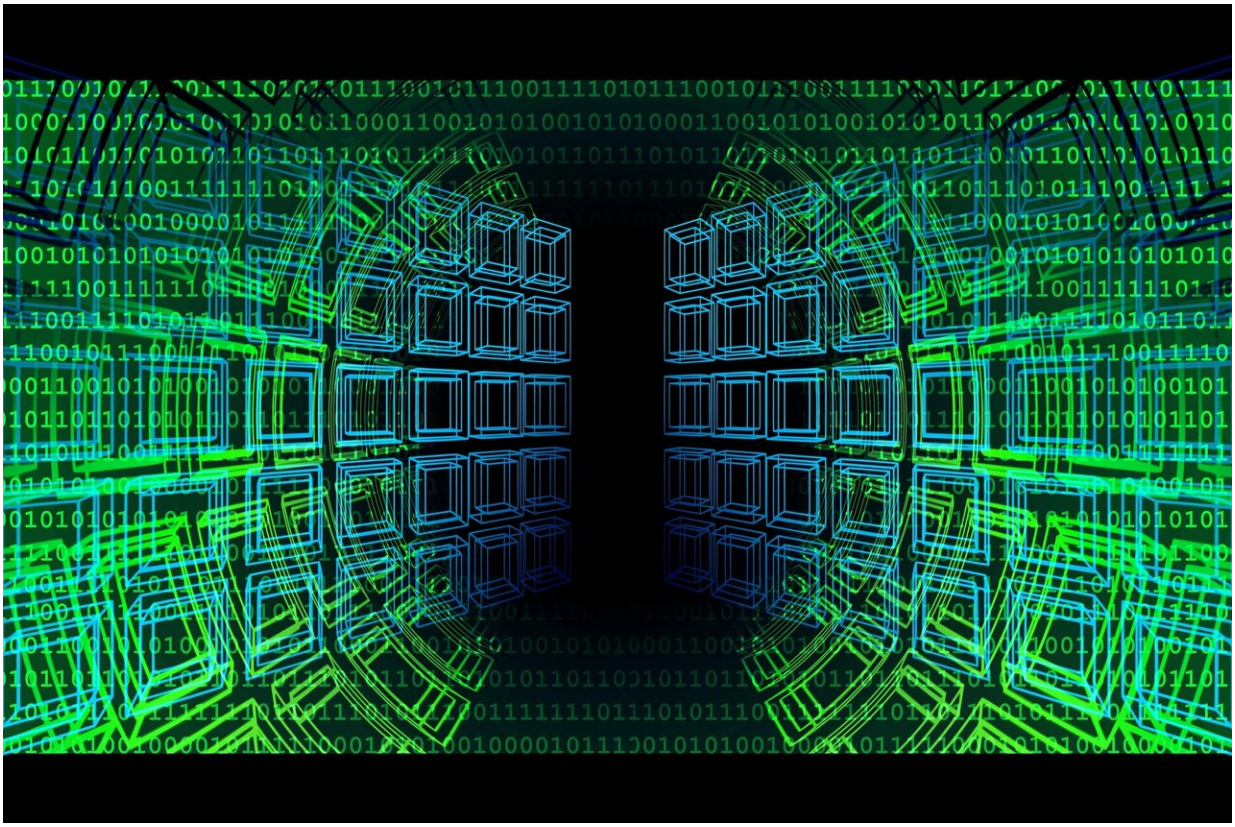

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To help keep first responders safe, University of Central Florida researchers have developed an artificial intelligence method that not only rapidly and remotely detects the powerful drug fentanyl, but also teaches

itself to detect any previously unknown derivatives made in clandestine batches.

The method, published recently in the journal *Scientific Reports*, uses infrared light spectroscopy and can be used in a portable, tabletop device.

"Fentanyl is a leading cause of drug overdose death in the U.S.," said Mengyu Xu, an assistant professor in UCF's Department of Statistics and Data Science and the study's lead author. "It and its derivatives have a low lethal dose and may lead to death of the user, could pose hazards for first responders and even be weaponized in an aerosol."

Fentanyl, which is 50 to 100 times more potent than morphine according to the U.S. Centers for Disease Control and Prevention, can be prescribed legally to treat patients who have severe pain, but it also is sometimes made and used illegally.

Subith Vasu, an associate professor in UCF's Department of Mechanical and Aerospace Engineering, co-led the study.

He said that rapid identification methods of both known and emerging opioid fentanyl substances can aid in the safety of law enforcement and military personnel who must minimize their contact with the substances.

"This AI algorithm will be used in a detection device we are building for the Defense Advanced Research Projects Agency," Vasu said.

For the study, the researchers used a national organic-molecules database to identify molecules that have at least one of the functional groups found in the parent compound fentanyl. From that data, they constructed machine-learning algorithms to identify those molecules based on their infrared spectral properties. Then they tested the accuracy of the

algorithms. The AI method had a 92.5 percent accuracy rate for correctly identifying molecules related to fentanyl.

Xu said this is the first time a systematical analysis has been conducted that identifies the fentanyl-related functional groups from infrared spectral data and uses tools of machine learning and statistical analysis.

Study co-author Chun-Hung Wang is a postdoctoral scholar in UCF's NanoScience Technology Center and helped study the compounds' spectral properties. He said identifying fentanyls is difficult as there are numerous formulations of analogs of fentanyl and carfentanil.

Artem Masunov, a co-author and an associate professor in UCF's NanoScience Technology Center and Department of Chemistry, investigated the functional groups that are common to the chemical structures of fentanyl and its analogs.

He said that despite differences in the analogs, they have common functional groups, which are structural similarities that enable the compounds to bind to receptors within the body and perform a similar function.

Anthony Terracciano, study co-author and a research engineer in UCF's Department of Mechanical and Aerospace Engineering, worked with Wang to examine the infrared spectra properties. He said profiling and analysis of infrared spectra is rapid, highly accurate, and can be done with a tabletop device.

The current research used infrared spectral data from compounds in gas form, but the researchers are working on a similar study to use machine-learning to detect fentanyl and its derivatives in powder form. The product of the technology is expected to be mature for practical on-site rapid identification by 2021.

More information: Mengyu Xu et al, High accuracy machine learning identification of fentanyl-relevant molecular compound classification via constituent functional group analysis, *Scientific Reports* (2020). DOI: 10.1038/s41598-020-70471-7

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