

# Novel software tool extracts important chemical exposure data

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Southwest Research Institute is introducing Floodlight, a novel software tool that efficiently discovers the vast numbers of chemical components—previously known and unknown—present in the food, air, drugs and products we are exposed to every day. This cheminformatics machine learning tool integrates algorithms with analytical chemistry software to provide deep analysis of gas chromatography mass spectrometry (GC/MS) and other instrument data.

GC/MS instruments identify different chemical substances within a test sample. Floodlight is a game changer for processing non-targeted analysis (NTA) data. NTA looks for any and all chemicals present in a sample, producing vast amounts of data. That's in contrast to targeted analyses, which look for a set of known [chemical elements](#), producing more limited results.

"Known chemicals in a particular sample are relatively easy to find and quantify," said Dr. Kristin Favela, an analytical chemist specializing in chemical forensics and environmental [chemistry](#). "NTA is a different story. Through an extensive, multiyear NTA program we discovered only about 20% of identified chemicals were included on the consumer product list. The remaining 80% were previously unidentified in these products.

"Consider the mysterious health effects we are seeing from e-cigarettes right now," Favela said. "Currently, the [medical community](#) does not know what's causing these serious problems, but based on our research,

there are likely unknown chemicals present in any given formula."

Today, the vast amount of NTA data collected requires careful examination by a chemist to identify and exclude data artifacts, flaws in the data caused by equipment, techniques or conditions. Automating this data quality review with Floodlight was necessary to develop a viable analytic process.

"The key to Floodlight is [artificial intelligence](#) and machine learning algorithms that enable advanced analysis of chemistry [big data](#)," said Dr. Keith Pickens, who led the SwRI team that fuses chemistry, data science and engineering expertise to home in on NTA. "Floodlight is a sophisticated software tool that can make sense of the vast amounts of data NTA generates."

SwRI is well positioned to attack this issue, with wide ranging expertise in analytic chemistry, machine learning, data science and engineering. Key to Floodlight is SwRI's development of a rapid analytical method to characterize chemicals in a wide array of consumers products, ranging from food and medicine to packaging and toys. SwRI used this data to train the algorithms.

Chemical data analysis is used in analytical chemistry, environmental testing and manufacturing. It provides the most valuable chemical information, helping guide the decision-making process within the chemical context. SwRI's chemical data analysis solutions range from [chemical](#) testing to data analysis and software development.

Provided by Southwest Research Institute

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