Researcher's computing testing could help identify toxic compounds

April 14 2014, by Cody Howard

Researchers at the University of Kansas School of Engineering are working on a new way to identify in advance whether a chemical could be toxic. Jun "Luke" Huan, associate professor of electrical engineering and computer science, uses an advanced computational method to analyze vast volumes of data on chemical compounds and determine which ones are more likely to cause complications in humans in small doses.

Based on data from the Environmental Protection Agency (EPA) and the Office of Toxic Substances, Huan estimates there are more than 100,000 chemicals that have not undergone simple toxicological experiments. A vast majority of these chemicals pose little or no threat to humans, especially in small doses. His research seeks to identify potential threats in a faster and less costly way than traditional methods.

"Testing toxicity of chemicals is expensive and time-consuming. It takes a lot of resources and creates ethical questions because traditional testing methods involve animal testing," said Huan, who is director of the Bioinformatics and Computational Life Sciences Laboratory at the Information and Telecommunication Technology Center. "The statistical algorithm we've developed helps identify which chemicals the EPA should prioritize and which ones are likely to be toxic so those can be tested first."

Huan's research on predicting the potential toxicity of chemical compounds was published in 2013 in the International Journal of Data

Mining and Bioinformatics and was featured in a July 2013 article in R&D Magazine. It was conducted as part of a five-year, $500,000 CAREER Award from the National Science Foundation, awarded in 2009 to further his work in bioinformatics. Bioinformatics harnesses computer analysis to learn more about complex biological information, especially molecular genetics and genomics.

As Huan's team collects and screens data on chemicals, they're working to create an open database that could serve as a valuable resource to any researcher interested in examining potential threats.

"We're trying to establish a platform so anyone can send us information, download data and access it freely. We're hoping to create a platform to help promote additional research," he said.

Provided by University of Kansas