

New algorithm allows for faster, animal-free chemical toxicity testing

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The use of animals to test the toxicity of chemicals may one day become outdated thanks to a low-cost, high-speed algorithm developed by researchers at Rutgers and other universities.

Toxicity testing—determining the amount of exposure to a [chemical](#) that is unsafe for humans—is vital to the safety of millions of workers in various industries. But of the 85,000 [compounds](#) used in consumer products, the majority have not been comprehensively tested for safety. Animal testing, in addition to its [ethical concerns](#), can be too costly and time consuming to meet this need, according to the study published in *Environmental Health Perspectives*.

"There is an urgent, worldwide need for an accurate, cost-effective and rapid way to test the [toxicity](#) of chemicals, in order to ensure the safety of the people who work with them and of the environments in which they are used," said lead researcher Daniel Russo, a doctoral candidate at the Rutgers University-Camden Center for Computational and Integrative Biology. "Animal testing alone cannot meet this need."

Previous efforts to solve this problem used computers to compare untested chemicals with structurally similar compounds whose toxicity is already known. But those methods were unable to assess structurally unique chemicals—and were confounded by the fact that some structurally similar chemicals have very different levels of toxicity.

The Rutgers-led group overcame these challenges by developing a first-of-its-kind [algorithm](#) that automatically extracts data from PubChem, a National Institutes of Health database of information on millions of chemicals. The algorithm compares chemical fragments from tested compounds with those of untested compounds, and uses multiple [mathematical methods](#) to evaluate their similarities and differences in order to predict an untested chemical's toxicity.

"The algorithm developed by Daniel and the Zhu laboratory mines massive amounts of data, and discerns relationships between fragments of compounds from different chemical classes, exponentially faster than a human could," said co-author Lauren Aleksunes, an associate professor at Rutgers' Ernest Mario School of Pharmacy and the Rutgers Environmental and Occupational Health Sciences Institute. "This model is efficient and provides companies and regulators with a tool to prioritize chemicals that may need more comprehensive testing in animals before use in commerce."

To fine-tune the algorithm, the researchers began with 7,385 compounds for which toxicity data is known, and compared it with data on the same chemicals in PubChem. They then tested the algorithm with 600 new compounds. For several groups of chemicals, the Rutgers-led algorithm had a 62 percent to 100 percent success rate in predicting their level of oral toxicity. And by comparing relationships between sets of chemicals, they shed light on new factors that can determine

the toxicity of a chemical.

Although the algorithm was directed only to assess the chemicals' level of toxicity when consumed orally, the Rutgers-led researchers conclude that their strategy can be extended to predict other types of toxicity.

"While the complete replacement of [animal testing](#) is still not feasible, this model takes an important step toward meeting the needs of industry, in which new chemicals are constantly under development, and for environmental and ecological safety," said the corresponding author Hao Zhu, an associate professor of chemistry at Rutgers-Camden and the Rutgers and Environmental and Occupational Health Sciences Institute.

More information: Daniel P. Russo et al, Nonanimal Models for Acute Toxicity Evaluations: Applying Data-Driven Profiling and Read-Across, *Environmental Health Perspectives* (2019). DOI: [10.1289/EHP3614](https://doi.org/10.1289/EHP3614)

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