

Public health researchers map world's 'chemical landscape'

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Researchers from the Johns Hopkins Bloomberg School of Public Health have created a map of the world's chemical landscape, a catalogue of 10,000 chemicals for which there is available safety data that they say can predict the toxicity of many of the 90,000 or more other substances in consumer products for which there is no such information.

The map, described online Feb. 12 in the journal *Alternatives to Animal Experiments* and being presented at the American Association for the Advancement of Science conference the same day in Washington, DC, was designed to help regulators, manufacturers and scientists get a good idea about whether chemicals for which there is little research are harmful or not. The research was done by creating a searchable database of the 816,000 research studies conducted on 10,000 chemicals registered in Europe, which includes information about whether they pose a hazard to humans and what type.

"There are 100,000 chemicals in products we use every day and we are missing 90 percent of the [safety information](#) we need," says study leader Thomas Hartung, MD, PhD, the Doerenkamp-Zbinden Professor and Chair for Evidence-based Toxicology at the Bloomberg School. "It would take billions of dollars to test every one of them which is very cost prohibitive. To address this, we have come up with a computer model that can tell us which chemicals are similar to untested ones to give us an idea of what types of hazards they are likely to pose."

The European Chemical Agency began registering chemical compounds

such as solvents, detergents, colorants and food additives in 2007, after legislation known as REACH stipulated the eventual collection of comprehensive safety information for all substances on the European market at more than one ton per year of production or sales volume. Korea and China also have similar rules and the United States and China are expected to follow suit, Hartung says.

Hartung's team took the studies submitted to the European Chemical Agency and made them into a [searchable database](#), characterizing in standardized text the known hazards of substances that have so far been registered. The team created a map, grouping chemicals by their known toxicities. The most prevalent hazards are that a chemical may cause an allergic skin reaction (20 percent), and causes serious eye damage (17 percent), but hazards include toxicity when inhaled or swallowed, flammability, organ damage and many more.

Since it would be virtually impossible to test every chemical, in lieu of prohibitively expensive testing, Hartung says an untested chemical could be entered into the computer map, next to all similar chemicals. If the chemical landed in a part of the map where similar chemicals are considered safe, that chemical could be deemed safe. If it landed in a place where its neighbors are, say, known to cause skin allergies, the chemical would be given that label. If a manufacturer protested that characterization, it could then do the testing necessary to try to prove that label wrong. If it falls in a gray area, testing would be needed.

This process of characterizing these untested chemicals is called "read-across." In parallel to developing this database, Hartung's group has steered a consensus process with 30 international experts, developing guidance on how to conduct a read-across. The consensus document is also being released Feb. 12 and will be discussed in dedicated conferences with experts in Brussels and Washington at the end of February.

Together, the availability of data and the know-how to exploit them is a powerful tool that could save millions of animals that researchers wouldn't have to use to test the safety of chemicals, Hartung says. The safety profile could come without any further animals harmed, he says.

"This is an extremely pragmatic system," says Hartung, who also directs the Center for Alternatives to Animal Testing at the Johns Hopkins Bloomberg School of Public Health. "You're never sure there's not going to be a surprise but this enormous database makes surprises much less likely. This database is a goldmine and will be made publicly available shortly."

Just because a chemical is deemed unsafe in certain ways doesn't mean it can't be used, Hartung notes. "If a tiger is in a cage, it's not harmful to you," he says. "It's the same with a [chemical](#). If you're not exposed, it's not a problem for you. So if you know something is corrosive to the skin, you need to take care not to use too much and to protect the skin. Knowledge can help you protect yourself."

Currently, the team is creating a spin-off company, to be called ToxTrack, which will make such analysis available as a web-based service.

"We want to make it possible that any substance - even a substance not yet synthesized - can be entered into the program and its possible safety problems can be predicted," Hartung says. "This could help in identifying the better substances to develop cleaner products or exchange those in common use with safer ones."

More information: "Global analysis of the publicly available safety data for 9,801 chemicals registered under the European REACH legislation from 2008-2014" *Alternatives to Animal Experiments*, 2016.

Provided by Johns Hopkins University Bloomberg School of Public Health

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