Researchers' novel tool to help develop safer pesticides

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The majority of commercial chemicals that enter the market in the United States every year have insufficient health and safety data. For pesticides, the U.S. Environmental Protection Agency uses a variety of techniques to fill data gaps in order to evaluate chemical hazard, exposure and risk. Nonetheless, public concern over the potential threat that these chemicals pose has grown in recent years, along with the

realization that traditional animal-testing methods are not pragmatic by means of speed, economics or ethics. Now, researchers at the George Washington University have developed a new computational approach to rapidly screen pesticides for safety, performance and how long they will endure in the environment. Moreover, and most importantly, the new approach will aid in the design of next-generation molecules to develop safer pesticides.

"In many ways, our tool mimics computational drug discovery, in which vast libraries of chemical compounds are screened for their efficacy and then tweaked to make them even more potent against specific therapeutic targets," Jakub Kostal, an assistant professor of chemistry at GW and principal investigator on the project, said. "Similarly, we use our systems-based approach to modify pesticides to make them less toxic and more degradable, while, at the same time, making sure they retain good performance. It's a powerful tool for both industry and regulatory agencies that can help design new, safer analogs of existing commercial agrochemicals, and so protect human life, the environment and industry's bottom line."

Using their model, the team analyzed 700 pesticides from the EPA's pesticide registry. The model considered a pesticide's likely persistence or degradation in the environment over time, its safety, and how well it performed at killing, repelling or controlling the target problem.

They found that only 52, or 7%, of the chemical compounds analyzed fulfilled the criteria for a safe chemical. According to the researchers, while the results from the analysis suggest most pesticides are likely not safe, many could be made safer by modifying their molecular structure in ways that would reduce their toxicity without sacrificing performance.

"Our analysis reveals there is definitely room for improvement when it comes to developing safer pesticides," Jessica Lewer, a graduate student

at GW and lead author on the paper, said. "Moreover, the computational approach we've developed to better screen and design safe pesticides can be used as a blueprint and applied to other industries that rely on commercial chemicals, for example cosmetics and cleaning products."

Going forward, the team hopes to augment their model with pesticide design from biobased, renewable chemical building blocks to advance sustainability goals in chemical design.

The study, "Structure-to-Process Design Framework for Developing Safer Pesticides," was published in the journal *Science Advances* on March 30, 2022.

More information: Jessica M. Lewer et al, Structure-to-process design framework for developing safer pesticides, *Science Advances* (2022). DOI: 10.1126/sciadv.abn2058.
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