

OSU researchers develop computer model to predict which pesticides will harm bees

By SIERRA DAWN McCLAIN
Capital Press

CORVALLIS, Ore. — Oregon State University researchers have developed a computer model that can predict if a pesticide will be harmful to honey bees.

The project involved training a machine learning model to predict whether any new proposed herbicide, fungicide or insecticide would be toxic to bees based on the compound's molecular structure.

"This research could be useful to other academics, researchers or companies exploring potential future pesticides," said Cory Simon, assistant professor of chemical engineering at Oregon State University.

With support from Simon and his co-researcher, Xiaoli Fern, associate professor of computer science at OSU, graduate students Ping Yang and Adrian Henle wrote computer codes and "trained" machine learning algorithms.

For this study, the researchers used an existing dataset containing 382 pesticide molecules for which honey bee toxicity outcomes were already known.

The researchers split this dataset in two. They used 80% of the molecules as a training set — using the data to train the machine learning algorithm to recognize patterns of toxicity by showing it examples.

The researchers used the remaining 20% to test how well the algorithm they had developed worked. For this test data set, they compared the algorithm's toxicity predictions against real data they already knew about toxicity.

The algorithm works by looking for common patterns or sequences that signal toxicity to bees using a mathematical concept called a "random walk."



Sierra Dawn McClain/Capital Press

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Xiaoli Fern



Adrian Henle



Ping Yang



Cory Simon

Simon describes a random walk like this: Imagine a tiny ant is taking a random stroll along a pesticide molecule's chemical structure, making its way from atom to atom along the bonds that hold the compound together. If that ant were then to visit another molecule and make another random journey, would it see a similar sequence of atoms and bonds? If so, then the two molecules are similar. And if one of those molecules is toxic to bees, the similar molecule also has a higher statistical likelihood

of being toxic to bees.

This method is the first of two ways OSU's new study represents the pesticide molecules. The second part of the study focuses on molecular access system, or MACCS, fingerprints, structure fingerprints that are used to measure molecular similarity.

This portion of the research involves looking for specific, pre-defined substructures and patterns in the molecules that are known to be predictive of the activity of drug molecules. Researchers look for

specific things, said Simon: "Is there a ring? Is there a chlorine atom? How about an amine group?" This, he said, gives an "interpretable" machine learning model.

Simon said researchers can use OSU's algorithm, in conjunction with other molecular models, to predict which pesticides are likely to be toxic to bees and therefore merit further study.

The scientist said he hopes OSU's work "can help (researchers) design effective pesticides that aren't toxic to bees."

More broadly, Simon said the use of data-driven molecular modeling and machine learning is "really burgeoning" and may play a larger role in pesticide development in the future.

"It's a really growing field," said Simon.

Railroad labor strike averted, for now

By SIERRA DAWN McCLAIN
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The Biden administration has intervened in railroad contract negotiations to block a strike for at least 60 days, temporarily averting what could have become a widespread work stoppage.

On July 15, Biden appointed a federal panel, consisting of third-party arbitrators, to help resolve the dispute over railroad worker wages and benefits.

"These disputes threaten substantially to interrupt interstate commerce to a degree that would deprive a section of the country of essential transportation service," Biden said in his executive order.

The intervention will keep about 115,000 rail workers on the job while arbitrators develop recommendations for both sides — railroad companies and unions — to consider.

Agricultural shippers are relieved that a potential strike has been forestalled.

According to an analysis of rail car data from the American Farm Bureau Federation, farmers are already experiencing rail order delays. In grain shipments, for example, between the second quarter of 2021 and second quarter of 2022, the cumulative number of unfilled grain car orders jumped 231%, and it's common for orders to arrive 11 or more days overdue. A rail strike could have further exacerbated delays.

The dispute is between Class I railroads, represented by the National Carriers Conference Committee, and two unions together representing 115,000 workers: the Coordinated Bargaining Coalition and the BMWED/SMART-MD Coalition.

Railroads, including BNSF Railway, CSX Transportation Inc., Union Pacific Railroad Co. and Norfolk

Southern Railway, have been in contract talks with unions since late 2019.

The railroads entered mediation with the BMWED/SMART-MD Coalition in June last year and with the Coordinated Bargaining Coalition in late January of this year.

On June 14, the National Mediation Board ended the mediation process, offering the parties a chance to submit their dispute to binding interest arbitration. The railroads accepted the offer; the unions declined.

Then union members voted to authorize a strike. The White House faced a July 17 deadline to intervene.

To prevent a July 18 strike, Biden appointed a three-member federal panel — called the Presidential Emergency Board — to try to broker an agreement between the railroads and unions. Panel members are Ira Jaffe, chair, and board members Barbara Deinhardt and David Twomey.

The National Carriers Conference Committee, representing the nation's freight railroads, said it is pleased that Biden appointed the arbitrators.

"All three are experienced, respected labor arbitrators with significant experience resolving labor disputes," said the NCCC.

The unions also applauded the move.

"We commend President Biden for announcing a board of neutral arbitrators to investigate and report its findings and recommendations to help both parties work toward a resolution," said the unions.

The panel has 30 days from July 15 to conduct hearings and issue its report, including settlement recommendations. During that time, a strike is not allowed. Work stoppages are also prohibited for another 30 days after the report is issued.



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