Peering into the mind of artificial intelligence to make better antibiotics

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Credit: American Chemical Society

Artificial intelligence (AI) has exploded in popularity. It powers models that help us drive vehicles, proofread emails and even design new molecules for medications. But just like a human, it's hard to read AI's mind.

Explainable AI (XAI), a subset of the technology, could help us do just that by justifying a model's decisions. And now, researchers are using

XAI to not only scrutinize predictive AI models more closely, but also to peer deeper into the field of chemistry.

The researchers present their results at the fall meeting of the American Chemical Society.

AI's vast number of uses has made it almost ubiquitous in today's technological landscape. However, many AI models are black boxes, meaning it's not clear exactly what steps are taken to produce a result. And when that result is something like a potential drug molecule, not understanding the steps might stir up skepticism with scientists and the public alike.

"As scientists, we like justification," explains Rebecca Davis, a chemistry professor at the University of Manitoba. "If we can come up with models that help provide some insight into how AI makes its decisions, it could potentially make scientists more comfortable with these methodologies."

One way to provide that justification is with XAI. These machine learning algorithms can help us see behind the scenes of AI decision making. Though XAI can be applied in a variety of contexts, Davis' research focuses on applying it to AI models for drug discovery, such as those used to predict new antibiotic candidates.

Considering that thousands of candidate molecules can be screened and rejected to approve just one new drug—and antibiotic resistance is a continuous threat to the efficacy of existing drugs—accurate and efficient prediction models are critical.

"I want to use XAI to better understand what information we need to teach computers chemistry," says Hunter Sturm, a graduate student in chemistry in Davis' lab who's presenting the work at the meeting.

The researchers started their work by feeding databases of known drug molecules into an AI model that would predict whether a compound would have a biological effect. Then, they used an XAI model developed by collaborator Pascal Friederich at Germany's Karlsruhe Institute of Technology to examine the specific parts of the drug molecules that led to the model's prediction.

This helped explain why a particular molecule had activity or not, according to the model, and that helped Davis and Sturm understand what an AI model might deem important and how it creates categories once it has examined many different compounds.

The researchers realized that XAI can see things that humans might have missed; it can consider far more variables and data points at once than a human brain. For example, when screening a set of penicillin molecules, the XAI found something interesting.

"Many chemists think of penicillin's core as the critical site for antibiotic activity," says Davis. "But that's not what the XAI saw." Instead, it identified structures attached to that core as the critical factor in its classification, not the core itself.

"This might be why some penicillin derivatives with that core show poor biological activity," explains Davis.

In addition to identifying important molecular structures, the researchers hope to use XAI to improve predictive AI models. "XAI shows us what computer algorithms define as important for antibiotic activity," explains Sturm.

"We can then use this information to train an AI model on what it's supposed to be looking for," Davis adds.

Next, the team will partner with a microbiology lab to synthesize and test some of the compounds the improved AI models predict would work as antibiotics. Ultimately, they hope XAI will help chemists create better, or perhaps entirely different, antibiotic compounds, which could help stem the tide of antibiotic-resistant pathogens.

"AI causes a lot of distrust and uncertainty in people. But if we can ask AI to explain what it's doing, there's a greater likelihood that this technology will be accepted," says Davis.

Sturm adds that he thinks AI applications in chemistry and drug discovery represent the future of the field. "Someone needs to lay the foundation. That's what I hope I'm doing."

More information: Using explainable artificial intelligence to explore the relationship between structure and activity, ACS Fall 2024.

Provided by American Chemical Society

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