News and Perspectives

Can AI Help Repurpose Drugs to Fight Against Antibiotic Resistance?

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Abstract

Drug repurposing and development to meet the threat of antimicrobial resistance can be costly and time-consuming, but AI models may be able to help. In this *News and Perspectives* article, JMIR Correspondent Sara Novak reports on recent research training models to identify candidate drugs to treat resistant infections.

Key Takeaways:

- Antibiotic resistance led to 4.7 million deaths globally in 2021.
- AI models can help identify drugs that can be repurposed for use in treating antibiotic-resistant infections, as well as to discover new drugs.
- Overhyping AI for use in drug discovery could lead to an overinvestment in AI companies that fall short on results.

Antimicrobial resistance (AMR) occurs when bacteria no longer respond to available antibiotics, leading to some infections becoming untreatable. According to the World Health Organization, bacterial AMR was responsible for up to 4.7 million deaths globally in 2021, and around 1 in 6 laboratory-confirmed infections were resistant in 2023.

In response to the growing threat, scientists are researching the use of AI models to identify drugs that can be repurposed to treat infections resistant to available antibiotics.

How AI Can Help Find New Uses for Old Drugs

Drug repurposing is particularly promising because it builds on existing, known drug profiles, allowing drug companies to skip the early stages of drug development that can be costly and time-intensive. Using AI can add further efficiency and cost-effectiveness.

"Drug repurposing is a good application for generative AI because it's able to leverage large amounts of safety and efficacy data that's already available," says James Zou, PhD, a biomedical data scientist at Stanford University.

AI algorithms are adept at analyzing large-scale datasets for drug responses to predict a smaller number of promising drugs that could be tested for potential repurposing, according to a review published last year in *Advanced Science*.

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> James Zou, PhD

Now, scientists are researching the use of AI for repurposing older drugs to treat *Streptococcus pneumoniae*, a widespread bacteria that can cause serious infections like pneumonia and bloodstream infections, as well as more minor ear and sinus infections. Strains of the bacteria with some degree of antibiotic resistance account for 40% of streptococcal infections in the United States.

Streptococcus pneumoniae has been particularly likely to develop resistance because once the bacteria is exposed to high levels of antibiotics, it's unusually adept at altering its DNA in ways that can make it more resistant to penicillin and other commonly used antibiotics.

While drug repurposing may not completely stop or prevent streptococcal bacteria from developing resistance, expanding our treatment options may help slow its impact. In another

Advanced Science study released in September this year, researchers used three different machine learning models to screen compounds to see if they could be repurposed for treatment of *Streptococcus pneumoniae*.

The models predicted that 11 potential drugs, whittled down from a whopping 6747 candidates, could be effective. Remarkably, 9 of these were shown in the lab to slow the growth of the bacteria.

Two drugs in particular, thiostrepton and ceftiofur—both antibiotics used in veterinary medicine—were found to be particularly potent tools for treating antibiotic-resistant *S pneumoniae*.

"AI models achieved an 81.8% prospective hit rate in repurposing drugs against an antibiotic-resistant strain of *Streptococcus pneumoniae*," says study author Pedro Ballester, PhD, an associate professor at Imperial College London and an expert in using AI for drug discovery.

Researchers contend that this success rate exceeds benchmarks and shows promise in an industry that's been estimated to spend up to US $2 billion on the development of a new drug.

Other research has been done on repurposing drugs for treatment of *Acinetobacter baumannii*, a serious bacteria, often found in hospital settings, that is responsible for 8000 resistant blood, urinary tract, lung, and wound infections annually.

Zou and his team trained an AI model to look for drugs that could be repurposed to inhibit the growth of the deadly bacteria.

Their model identified 70 compounds most likely to inhibit the bacteria and worked with the Ukrainian chemical company Enamine to synthesize the 6 most potent compounds—which were later found to be effective at killing *Acinetobacter baumannii*.

Using AI for Drug Discovery

Not only is there potential for AI models to be used in drug repurposing, drug development in general may also be a good target for AI algorithms. In 2025, Zou, along with Stanford University graduate student Harrison Zhang, established a virtual lab to mimic a traditional drug discovery company.

The "Virtual Biotech" consisted of over 37,000 AI agents who emulated the roles and organizational chart of a traditional drug company. For example, one division of AI agents looked at drug safety while another looked at drug efficacy, another at drug repurposing, and another at designing clinical trials, all of which you would expect in a traditional drug company.

Zou and his team also designed COVID nanobodies, antibodies that attack SARS-CoV-2 spike proteins and were validated to be effective in labs, using computational drug repurposing.

"One of the reasons that drug discovery is so expensive is because there are so many aspects that need to be considered to understand the biology, chemistry, and safety profile, as well as the commercial landscape," said Zou.

But in the virtual company, AI agents can systematically look across different sources of evidence in everything from patents to Food and Drug Administration (FDA) submissions, as well as the basic biology of the molecules, and then share that data among each other to do high-level computational analyses.

As an example of this application, Zou and his team directed AI agents to look at whether this virtual biotech company could design a drug—mirroring what a traditional drug company can do—in a shorter period of time. The virtual company identified a mechanism that allowed lung cancer tumors to evade chemotherapy and then designed a drug that homes in on the cancer cells and delivers a toxic chemotherapy load directly to them.

A few months later, Zou says, the pharmaceutical company Merck independently arrived at the same antibody-drug conjugate, and the treatment received an FDA breakthrough therapy designation, which speeds up trials for drugs that are needed to treat the most deadly of diseases.

A Word of Caution on the Hype

While there's a lot of excitement around using AI in drug repurposing and discovery, some researchers aren't so convinced. Critics contend that within the drug discovery world, the use of AI has been overhyped, leading to significant commercial investments in AI that may not deliver.

As of yet, not a single AI-discovered drug has received full FDA approval—even if the earlier stages of research can be fast-tracked with AI, the later stages, involving human subjects, still take time. And speed does not necessarily equal accuracy.

"The labs doing this work responsibly are the ones pairing AI hypotheses with real experimental validation, not mistaking faster outputs for deeper insight," noted Marinka Zitnik, associate professor in the Department of Biomedical Informatics at Harvard Medical School, in a recent Forbes article.

Ultimately, both speed and accuracy—and human and artificial intelligence—will be necessary to tackle AMR.

Keywords: anti-bacterial agents; drug discovery; drug repurposing; drug resistance; microbial; artificial intelligence; machine learning; computational biology; anti-infective agents

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