PROJECT MANAGEMENT GLOBAL
The Place for People in Projects

Scientists Use Generative AI to Design New Drugs That Combat Drug-Resistant Bacteria

September 2, 2025

Researchers from MIT have used generative artificial intelligence (AI) to design a new class of antibiotics capable of killing two difficult-to-treat infections: drug-resistant Neisseria gonorrhoeae and multi-drug-resistant Staphylococcus aureus (MRSA).

The research team used generative AI algorithms to create over 36 million possible compounds. After computationally screening them for antimicrobial properties, they found top candidates that are structurally different from any existing antibiotics. These new compounds appear to work by disrupting bacterial cell membranes through novel mechanisms, a strategy that could be applied to identify drugs against other species of bacteria.

James Collins, a professor at MIT and senior author of the study, said: “We’re excited about the new possibilities that this project opens up for antibiotics development. Our work shows the power of AI from a drug design standpoint, and enables us to exploit much larger chemical spaces that were previously inaccessible.”

The findings were published in the journal *Cell*.

Exploring New Chemical Territory

Over the last 45 years, the majority of new antibiotics have been variants of existing drugs, while bacterial resistance has continued to grow. Globally, it is estimated that drug-resistant bacterial infections cause nearly **5 million deaths per year**.

To combat this, the **Antibiotics-AI Project** at MIT has previously used AI to screen huge libraries of existing chemical compounds, leading to the discovery of promising candidates such as **halicin** and **abaucin**. In this new study, the researchers decided to expand their search into hypothetically possible molecules that don't exist in any known chemical libraries.

The researchers used two different generative AI approaches. In the first approach, they focused on designing molecules to kill *N. gonorrhoeae*, a bacterium that causes gonorrhoea. They began with a known chemical fragment that showed antimicrobial activity and used it as a basis for the AI to generate new compounds. This process yielded a promising compound named **NG1**, which proved effective at killing the bacterium in a lab dish and in a mouse model of the infection. Further experiments revealed that NG1 works by interfering with the synthesis of the bacterial outer membrane, a novel drug target.

In the second study, the researchers used the AI to freely design molecules to target **MRSA**. This time, the AI generated more than 29 million compounds with no constraints other than the general rules of chemistry. After filtering the pool, they found six molecules that showed strong antibacterial activity. The top candidate, named **DN1**, was able to clear a MRSA skin infection in a mouse model. These molecules also appear to interfere with bacterial cell membranes.

The non-profit organisation **Phare Bio**, which is also part of the Antibiotics-AI Project, is now working on further modifying NG1 and DN1 for additional testing. The researchers also plan to apply their AI platforms to other bacterial pathogens, including *Mycobacterium tuberculosis* and *Pseudomonas aeruginosa*.

Image: MIT