

Scientists use AI to discover new antibiotic to treat deadly superbug

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Scientists using artificial intelligence have discovered a new antibiotic that can kill a deadly superbug. According to a new study published on Thursday in the science journal *Nature Chemical Biology*, a group of scientists from McMaster University and the Massachusetts Institute of Technology have discovered a new antibiotic that can be used to kill a deadly hospital superbug. The superbug in question is *Acinetobacter baumannii*, which the World Health Organization has classified as a “critical” threat among its “priority pathogens” – a group of bacteria families that pose the “greatest threat” to human health. According to the WHO, the bacteria have built-in abilities to find new ways to resist treatment and can pass along genetic material that allows other bacteria to become drug-resistant as well. *A. baumannii* poses a threat to hospitals, nursing homes and patients who require ventilators and blood catheters, as well as those who have open wounds from surgeries. The bacteria can live for prolonged periods of time on environmental surfaces and shared equipment, and can often be spread through contaminated hands. In addition to blood infections, *A. baumannii* can cause infections in urinary tracts and lungs. According to the Centers for Disease Control and Prevention, the bacteria can also “colonize” or live in a patient without causing infections or symptoms. Thursday’s study revealed that researchers used an AI algorithm to screen thousands of antibacterial molecules in an attempt to predict new structural classes. As a result of the AI screening, researchers were able to identify a new antibacterial compound which they named abaucin. “We had a whole bunch of data that was just telling us about which chemicals were able to kill a bunch of bacteria and which ones weren’t. My job was to train this model, and all that this model was going to be doing is telling us essentially if new molecules will have antibacterial properties or not,” said Gary Liu, a graduate student from McMaster University who worked on the research. “Then basically through that, we’re able to just increase the efficiency of the drug discovery pipeline and ... hone in on all the molecules that we really want to care about,” he added. After scientists trained the AI model, they used it to analyze 6,680 compounds that it had previously not encountered. The analysis took an hour and a half and ended up producing several hundred compounds, 240 of which were then tested in a laboratory. Laboratory testing ultimately revealed nine potential antibiotics, including abaucin. The scientists then tested the new molecule against *A. baumannii* in a wound infection model in mice and found that the molecule suppressed the infection. “This work validates the benefits of machine learning in the search for new antibiotics” said Jonathan Stokes, an assistant professor at McMaster University’s department of biomedicine and biochemistry who helped lead the study. “Using AI, we can rapidly explore vast regions of chemical space, significantly increasing the chances of discovering fundamentally new antibacterial molecules,” he said. “We know broad-spectrum antibiotics are suboptimal and that

pathogens have the ability to evolve and adjust to every trick we throw at them ... AI methods afford us the opportunity to vastly increase the rate at which we discover new antibiotics, and we can do it at a reduced cost. This is an important avenue of exploration for new antibiotic drugs," he added.