

## Scientists Discover First New Antibiotic in Six Decades



A ground-breaking class of antibiotics targeting drug-resistant Staphylococcus aureus (MRSA) bacteria has been discovered by applying transparent deep-learning models in medicine. Artificial intelligence (AI) is revolutionising the field, aiding scientists in unveiling the first novel antibiotics in six decades.

Designated a priority-one critical pathogen by the World Health Organization, this organism has the potential to induce severe invasive blood and chest infections in critically ill hospital patients. It also exhibits resistance to numerous commonly used antibiotics.

Identifying a new compound capable of combatting a drug-resistant bacterium responsible for thousands of global deaths annually marks a pivotal moment in the battle against antibiotic resistance.

The findings, published in *Nature* and co-authored by a team of 21 researchers, employed a deep-learning model to predict the activity and toxicity of the innovative compound. Using artificial neural networks to autonomously learn features from data, deep learning is increasingly employed in drug discovery to expedite identification, predict properties, and optimise development processes.

Through an extensively enlarged deep learning model trained with expanded datasets, the researchers evaluated approximately 39,000 compounds for antibiotic activity against MRSA. Subsequently, integrating toxicity assessments on human cells, the researchers identified compounds effective against MRSA with minimal harm to the human body from a pool of around 12 million commercially available compounds.

The models revealed compounds from five distinct classes, based on specific chemical substructures, showing predicted activity against MRSA. Further experiments in laboratory settings confirmed the efficacy of two promising antibiotic candidates from the same class, with significant reductions in MRSA populations observed in mouse models for both skin and systemic infections.

The recently developed compound, zosurabalpin, demonstrated exceptional efficacy in both test tubes and mice. The study presents promising prospects for addressing challenging-to-treat infections. Zosurabalpin disrupts the organism's capability to effectively construct a vital protective membrane. Through laboratory trials, the compound effectively halted the transportation of a crucial building block, a lipopolysaccharide, to the outer cell, impeding the proper formation of the protective membrane and ultimately causing cell death.

The researchers have concluded initial first-in-man studies involving a relatively small group of healthy individuals. They are now prepared to progress to comprehensive clinical trials involving people with the infection. Nevertheless, there is still a long way to go before its potential use in hospitals.

Source: <u>BBC</u>, <u>Euronews</u>
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