HealthManagement
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AI Model to Design New Superbug-Fighting Antibiotics

Image caption: McMaster University's Jonathan Stokes is one of the researchers who developed a new generative AI model which can design new antibiotics to stop the spread of one of the world's most dangerous antibiotic-resistant bacteria.

A groundbreaking artificial intelligence model has been developed jointly by researchers from McMaster University and Stanford University. It aims to address the pressing need for novel antibiotics amidst the global challenge of drug-resistant bacteria. The innovative model, known as SyntheMol, can conceive billions of antibiotic molecules that are cost-effective and feasible for laboratory synthesis. Findings are published in Nature Machine Intelligence.

The global proliferation of drug-resistant bacteria has underscored the critical necessity for novel antibiotics. However, contemporary AI techniques face constraints in efficiently pinpointing potential chemical compounds, particularly as researchers concurrently tackle the challenges of synthesising and laboratory testing these AI-driven molecules.

The proliferation of drug-resistant bacterial strains, such as Acinetobacter baumannii, underscores the urgency for innovative solutions in antibiotic discovery. The study unveils SyntheMol's capability to target A. baumannii, identified by the World Health Organization as the world's most dangerous antibiotic-resistant bacteria, responsible for severe infections like pneumonia and meningitis.

Study researchers highlight the unique challenge posed by bacterial evolution, emphasising the imperative for a continuous supply of effective antibiotics. Leveraging artificial intelligence, particularly SyntheMol, researchers can swiftly and affordably sift through vast molecular landscapes to identify potential antibiotic candidates.

The methodology behind SyntheMol involves a comprehensive exploration of molecular fragments, akin to assembling Lego pieces, in conjunction with various chemical reactions. This approach yields an extensive array of candidate molecules with promising antibacterial properties, totalling 30 billion combinations. Moreover, SyntheMol incorporates an additional AI model to assess toxicity, identifying six non-toxic molecules demonstrating potent antibacterial activity against A. baumannii.

The new AI model generates novel antibiotic candidates and provides synthetic recipes for their production—a groundbreaking advancement as traditional chemists often lack the knowledge to synthesise AI-designed molecules. This type of advancement and innovative approaches can help combat antibiotic resistance.

Source: McMaster University

Image Credit: McMaster University

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