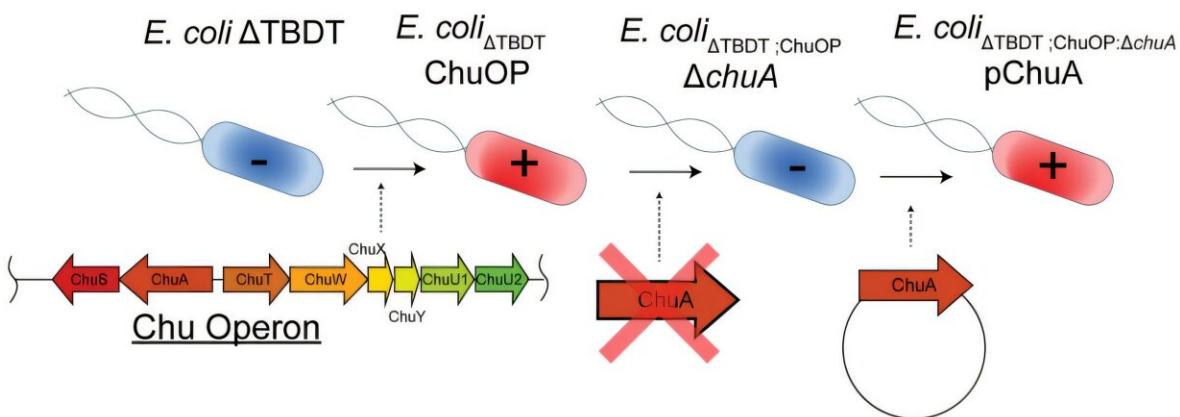# Scientists use AI to create protein that kills E. coli

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a) Schematic of the genetic engineering strategy for the generation of the ChuA reporter strain used in this study. Credit: *BioRxiv* (2024). DOI: 10.1101/2024.12.05.626953

In the last year, there has been a surge in proteins developed by AI that will eventually be used in the treatment of everything from snakebites to cancer. What would normally take decades for a scientist to create—a custom-made protein for a particular disease—can now be done in seconds.

For the first time, Australian scientists have used Artificial Intelligence (AI) to generate a ready-to-use biological protein, in this case, one that can kill antibiotic-resistant bacteria like E. coli.

This study, published in *Nature Communications*, provides a new way to combat the growing crisis caused by antibiotic-resistant superbugs.

By using AI in this way, Australian science has now joined countries like the US and China in having developed AI platforms capable of rapidly generating thousands of ready-to-use proteins, paving the way for faster, more affordable drug development and diagnostics that could transform biomedical research and patient care.

The paper is co-led by Dr. Rhys Grinter and Associate Professor Gavin Knott, a Snow Medical Fellow, who lead the new AI Protein Design Program with nodes at the University of Melbourne Bio21 Institute and Monash Biomedicine Discovery Institute.

According to Dr. Grinter and A/Prof. Knott, the AI Protein Design Platform used in this work, is the first in Australia that models the work done by David Baker (who won the Nobel Prize in Chemistry last year), developing an end-to-end approach that could create a wide range of proteins.

"These proteins are now being developed as pharmaceuticals, vaccines, nanomaterials and tiny sensors, with many other applications yet to be tested," Associate Professor Knott said.

For this study, the AI Protein Design Platform used AI-driven protein design tools that are freely available for scientists everywhere. "It's important to democratize protein design so that the whole world has the ability to leverage these tools," said Daniel Fox, the Ph.D. student who performed most of the experimental work for the study.

"Using these tools and those we are developing in-house, we can engineer proteins to bind a specific target site or ligand, as inhibitors, agonists or antagonists, or engineered enzymes with improved activity

and stability."

According to Dr. Grinter, currently, proteins used in the treatment of diseases like cancer or infections are derived from nature and repurposed through rational design or in vitro evolution and selection.

"These new methods in deep learning enable efficient de novo design of proteins with specific characteristics and functions, lowering the cost and accelerating the development of novel protein binders and engineered enzymes," he said.

Since the work of David Baker, new tools and software are being developed, such as Bindcraft and Chai, which have been incorporated into an AI Protein Design Platform co-led by Dr. Grinter and A/Prof. Knott.

Professor John Carroll, Director of the Monash Biomedicine Discovery Institute, said the new AI Protein Design Program brings Australia "right up to speed in this exciting new modality for designing novel therapeutics and research tools. It is testament to the entrepreneurial spirit of two fabulous young scientists who have worked night and day to build this capability from scratch."

"The Program, based at Monash University and the University of Melbourne, is run by a team of talented structural biologists and computer scientists who understand the design process from end-to-end. This in-depth knowledge of protein structure and machine learning makes us a highly agile program capable of regularly onboarding cutting-edge tools in AI-protein design," Associate Professor Knott said.

More information: Inhibiting heme piracy by pathogenic Escherichia coli using de novo-1 designed proteins, *Nature Communications* (2025). DOI: 10.1038/s41467-025-60612-9 On *BioRxiv*. DOI: