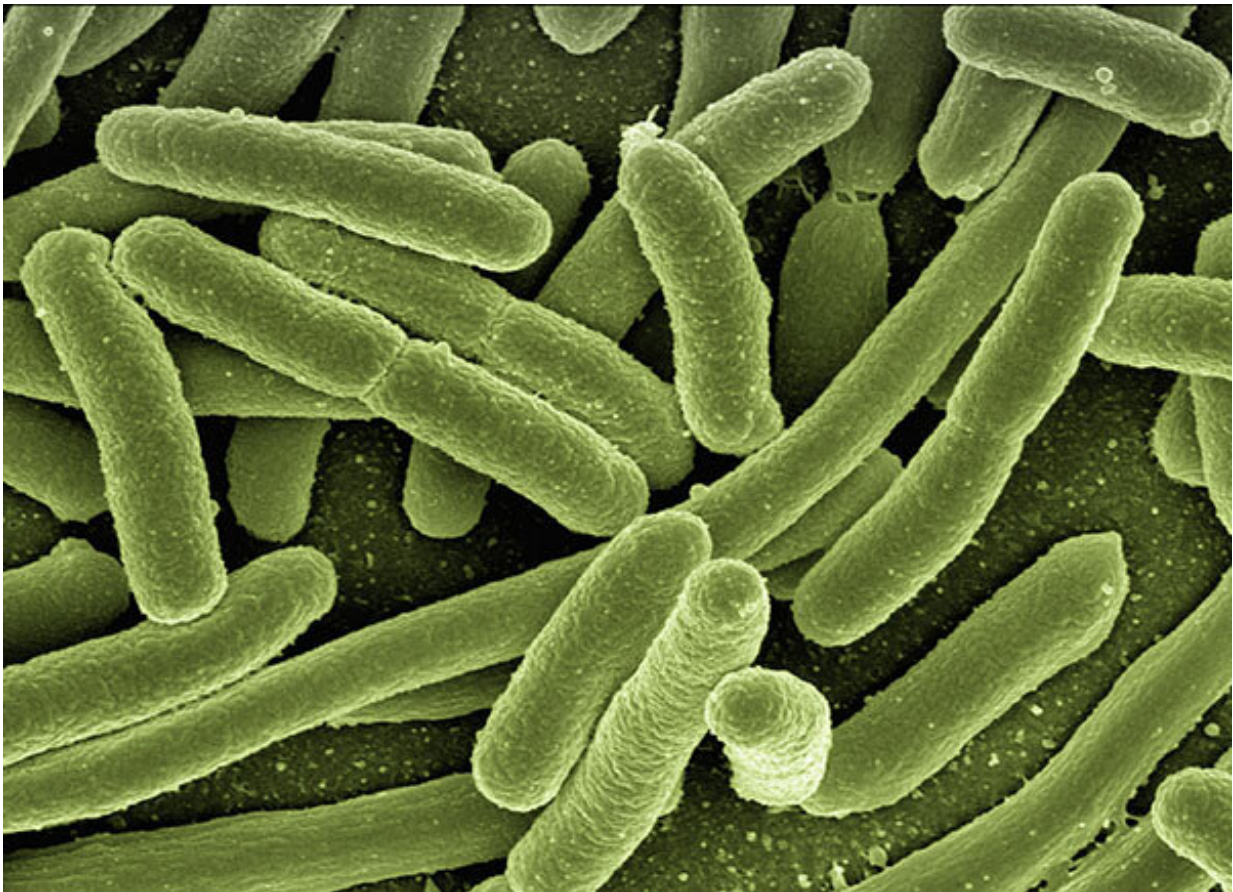


Antibiotic resistance outwitted by supercomputers

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Escherichia coli, one of the top three pathogens on World Health Organisation's target list. Credit: University of Portsmouth

Scientists may have made a giant leap in fighting the biggest threat to

human health by using supercomputing to keep pace with the impressive ability of diseases to evolve.

A new study by an international team, co-led by Dr. Gerhard Koenig from the University of Portsmouth, tackled the problem of antibiotic [resistance](#) by redesigning existing antibiotics to overcome bacterial resistance mechanisms.

About 700,000 people are estimated to die every year because of [antibiotic resistant bacteria](#), and that number is expected to rise to millions.

Without effective antibiotics, life expectancy is predicted to drop by 20 years.

The race has been on for many years to develop new [antibiotics](#) to fight disease faster than a disease can evolve.

Computers have been used in drug design for decades, but this is the first study to use a multi-pronged computer-guided strategy to make a new antibiotic from an existing one which [bacteria](#) have outwitted.

The research is published in *PNAS*.

Dr. Koenig, a computational chemist in the university's School of Biological Sciences, and first author on the paper, said: "Antibiotics are one of the pillars of modern medicine and antibiotic resistance is one of the biggest threats to human health. There's an urgent need to develop new ways of fighting ever-evolving bacteria.

"It's only a matter of time until bacteria develop counterstrategies against our counterstrategies and become resistant to the new antibiotic, so we will have to keep on studying bacterial resistance mechanisms and

develop new derivatives accordingly."

The hope of this new work lies in showing that the resistance mechanisms of bacteria can be addressed in a systematic way, allowing science to continually fight back with a computational evolution of [new antibiotics](#).

Dr. Koenig said: "Our computers are becoming faster with every year. So, there is some hope that we will be able to turn the tide.

"If computers can beat the world champion in chess, I don't see why they should not also be able to defeat bacteria."

The international team, including Nobel Prize laureate Ada Yonath, carried out the research at the Max-Planck-Institut für Kohlenforschung, the Weizmann Institute, and the universities of Duisburg-Essen, Bochum and Queensland.

They developed a strategy to simulate many aspects of a redesigned antibiotic at the same time, including how soluble it is, how effective it is at entering into the bacteria, and how efficient it is at blocking their protein production.

The computational work outlined in the research was done in a matter of weeks on one of the top supercomputers in Europe, but it took the international team several years to verify experimentally that their approach was indeed correct.

Dr. Koenig said: "Using a computational approach makes the development of new antibiotic derivatives faster and cheaper, and predicting whether a chemical compound is going to be active before it is synthesized also avoids chemical waste.

"This is an extremely empowering technology."

More information: Rational prioritization strategy allows the design of macrolide derivatives that overcome antibiotic resistance, *PNAS* (2021). doi.org/10.1073/pnas.2113632118

Provided by University of Portsmouth

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