

Press Release

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€ 1.18 million in funding for the ANTARES project

Combating resistance with artificial intelligence: Faster search for new antibacterial agents

Faster identification of new antibiotic candidates with the help of artificial intelligence: This is the goal of the research project ANTARES, funded by the German Federal Ministry for Research, Technology and Space (BMFTR). The Fraunhofer Institute for Translational Medicine and Pharmacology ITMP is collaborating with the Helmholtz Center for Infection Research (HZI) in Braunschweig and Enamine Germany GmbH in Frankfurt am Main (Enamine) to identify new, safe, and affordable treatment options for patients suffering from life-threatening and often drug-resistant infections.

Many bacterial pathogens are developing resistance to antibiotics. However, the development of new antibacterial agents is complex and expensive. The required substances are often chemically difficult to access, yet they must be tested in large quantities even in the early stages of research. This is exactly where the ANTARES research project comes in. With the help of artificial intelligence, antibacterial agents should be developed not only faster but also more cost-effectively. The consortium is guided by the analysis of specific bacterial species for which, according to the World Health Organization (WHO), new treatment options are particularly urgently needed.

The AI models used for this purpose are initially trained and tested on publicly available data sets. This makes it possible to find out early on and with low risk which models are particularly suitable. Subsequently, they are further developed using high-throughput tests with substances that are attributed with antibiotic activity. In this way, the research team improves prediction accuracy step by step. To further increase precision, not only are the antibiotics predicted by the AI as effective experimentally verified, but structurally similar compounds that the model initially classifies as inactive are also specifically tested. In a later step, the researchers then examine whether the identified active substances can also be used against resistant pathogens. "Particularly interesting is the question of whether new substances are either effective on their own or can make existing antibiotics effective again in combination. Such combination approaches are considered promising to increase the effectiveness of treatments and slow down the development of further resistance," explains consortium leader Dr. Bernhard Ellinger from Fraunhofer ITMP. "We initially work with known data sets, but we can also create and test newly synthesized substance libraries beyond that."

Repeated cycles of prediction and experimental validation of the AI models are an innovative approach of the project

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While other research programs often rely on a single training run of the model followed by validation, ANTARES focuses on repeated cycles of prediction and experimental verification of the trained AI models. For this purpose, the structure-activity relationships derived from the models are extracted using Explainable AI (XAI) approaches. In the next step, a generative model will propose new structures with antibiotic activity. The models and the developed standardized datasets will be published in accordance with the FAIR principles to support the further development of new antibiotics. "Our goal is to achieve time savings and a higher success rate in the discovery phase by combining AI with high-throughput experiments. To increase the value of the identified active molecules, we will also describe their mechanism of action and their spectrum of activity," explains Prof. Mark Brönstrup from the Helmholtz Centre for Infection Research, describing the motivation behind the research project.

Dr. Sven Wagner, Vice President for Partnerships at Enamine, assesses the significance of the project for the pharmaceutical industry: "We are facing a severe structural crisis worldwide in the development of urgently needed new antibiotics – the so-called 'broken market'. The fight against antimicrobial resistance (AMR) is of critical importance, yet the return on investment (ROI) for drug developers is vanishingly small. Enamine has made it its mission to support research in these areas of high medical need but low industrial interest. We want to bridge this 'valley of death' through crucial public-private partnerships. Within the ANTARES project, Enamine is driving forward the development and production of small-molecule active substances for antibiotic research on a larger scale."

Focus on bacteria with particularly urgent treatment needs

The research project focuses on particularly relevant pathogens that the World Health Organization has classified as critical. These bacterial species include, among others, *Acinetobacter baumannii*, *Escherichia coli*, and *Pseudomonas aeruginosa*. *Pseudomonas*, for example, can cause severe pneumonia. Especially in the lungs, treatment with antibiotics is often particularly difficult because the organ is hard to reach for many active substances. In addition, bacterial pathogens from the food chain are becoming increasingly important.

The project follows these bacterial groups identified by the WHO and works with selected, medically relevant pathogens. It is important to note that many priority lists refer primarily to resistant bacterial strains. However, for training the AI models, there is often more data available on non-resistant wild types so far. Therefore, the models are initially developed and experimentally tested based on such datasets.

About ANTARES

Title: Antibiotic Network for Targeted AI-driven Research and Explainable Screening (Acronym: ANTARES)

Start of the project: 01.07.2026

Project duration: 3 years

Grant amount: €1.18 million **Funded by: Federal Ministry of Research, Technology and Space (BMFTR)**

Research consortium: Enamine Germany GmbH, Fraunhofer Institute for Translational Medicine and Pharmacology ITMP, Helmholtz Centre for Infection Research

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