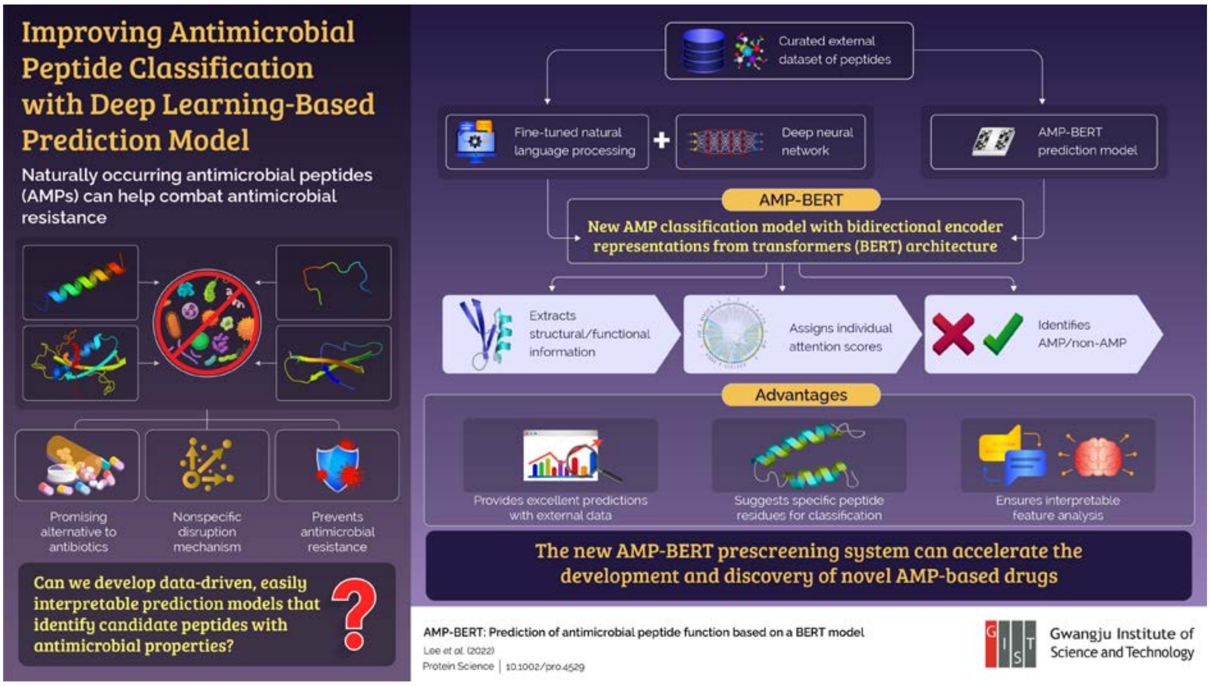
PRESS RELEASE

GIST Researchers Develop “AMP-BERT”: A New AI-based “Finder” of Antimicrobial Peptides

Scientists propose a deep neural network-based platform for identifying candidate antimicrobial peptides

Antimicrobial peptides (AMPs) are a promising new weapon for combating the growing antimicrobial resistance of bacteria and other harmful microorganisms. Now, researchers at the Gwangju Institute of Science and Technology developed a new, easily interpretable AI-powered prediction model named AMP-BERT that can capture the functional and structural properties of peptides and classify them as AMPs or non-AMPs. This study is a major step towards the acceleration of AMP-based drug discovery and therapeutics.



Improving Antimicrobial Peptide Classification with Deep Learning-Based Prediction Model

Naturally occurring antimicrobial peptides (AMPs) can help combat antimicrobial resistance

Can we develop data-driven, easily interpretable prediction models that identify candidate peptides with antimicrobial properties?

AMP-BERT: New AMP classification model with bidirectional encoder representations from transformers (BERT) architecture

The new AMP-BERT prescreening system can accelerate the development and discovery of novel AMP-based drugs

AMP-BERT: Prediction of antimicrobial peptide function based on a BERT model
Lee et al. (2022)
Protein Science | 10.1002/pro.4529

Image title: AMP-BERT provides an all-new deep learning approach to antimicrobial peptide discovery
Image Caption: Researchers from GIST developed natural language processing (NLP) and machine learning (ML)-based antimicrobial peptide (AMP) prediction model that can identify functional/structural properties of peptides and classify them as AMPs or non-AMPs.
Credit: Hojung Nam from the Gwangju Institute of Science and Technology
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Over the past few decades, antimicrobial resistance has become a major public health concern globally. This has led to a search for alternative methods of treating microbial infections. One such innovation is the discovery of antimicrobial properties of certain peptides. Antimicrobial peptides (AMPs) are short peptides found in most animals, plants, and microorganisms and act as a natural defense against infections. AMPs combat harmful bacteria via a non-specific mechanism that prevents them from developing resistance. Despite these exceptional abilities, research on AMPs is difficult because existing systems for identifying candidate AMPs are like a black box, where the outputs are not easily interpretable for further analysis.

Now, in a recent breakthrough published in *Protein Science,* a team of researchers from the Gwangju Institute of Science and Technology, including Prof. Hojung Nam and Mr. Hansol Lee, proposed an AMP-BERT classification system that uses AI-based bidirectional encoder representation from transformers (BERT) architecture to improve upon existing AMP classification models. Their findings were published online on 3 December 2022 and in print in Volume 32, Issue 1 of the journal in January 2023.

When asked about the motivation behind developing the classification system, Prof. Nam explains: "*The misuse and overuse of antibiotics have resulted in the development of bacteria that cannot be effectively treated with these antibiotics. This has resulted in an increased health risk not only in humans but also agriculture. So, we wanted to develop an AMP pre-screening platform that isn't a black box of algorithms but can be easily interpreted for further research.*"

The team incorporated a natural language processing (NLP)-based deep neural network that was pre-trained with billions of protein sequences that was then fine-tuned with thousands of peptide sequences from a benchmark AMP database. This enabled the AMP-BERT model to not only extract the structural and functional information from the input peptide sequences but also differentiate AMPs from non-AMPs. This enhanced the prediction power and allowed the model to make better classifications even with external data.

The team also designed the model to assign individual attention scores to each amino acid from the input peptide sequence. The attention feature then revealed the important subregions of AMPs that play a major role in determining whether a peptide has antimicrobial properties or not. Furthermore, the prediction results indicated the AMP-BERT model's applicability extends even to unseen peptide data and that it can learn meaningful functional and structural information from those peptides.

This novel AMP-BERT peptide pre-screening model can open new doors for the discovery and development of AMP-based drug candidates for treating antimicrobial-resistant illnesses. The important peptide subregion information provided by this prediction platform can also be used to optimize the antibiotic efficiency of peptides. "*As more AMPs are experimentally validated and new structural information is uncovered using computational methods, we will be able to make more effective antibiotic drugs and potentially stop a new pandemic from spreading across the world in near future*" concludes Prof. Nam.

AMP-BERT will certainly be a powerful weapon in our war against antimicrobial resistance!

Reference

Authors:	Hansol Lee[1] , Songyeon Lee[1] , Ingoo Lee[1] , Hojung Nam[1,2]
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About the Gwangju Institute of Science and Technology (GIST)

The Gwangju Institute of Science and Technology (GIST) is a research-oriented university situated in Gwangju, South Korea. Founded in 1993, GIST has become one of the most prestigious schools in South Korea. The university aims to create a strong research environment to spur advancements in science and technology and to promote collaboration between international and domestic research programs. With its motto of "A Proud Creator of Future Science and Technology," GIST has consistently received one of the highest university rankings in Korea.

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About the author

Hojung Nam is an Associate Professor in the School of Electrical Engineering and Computer Science, and the AI Graduate School at the Gwangju Institute of Science and Technology (GIST). She received her Ph.D. in the Dept. of Bio and Brain Engineering at the Korea Advanced Institute of Science and Technology (KAIST) and completed her postdoctoral training in the Dept. of Bioengineering at the University of California, San Diego (UCSD). Currently, her research group is working on the development of various computational tools for drug discovery, development, and models for the prediction of drug side effects.

Hansol Lee is a Ph.D. candidate at GIST under Prof. Hojung Nam's instruction. During his Ph.D. course, he has carried out research on AMP-related deep learning models, including AMP class prediction and AMP sequence generation.