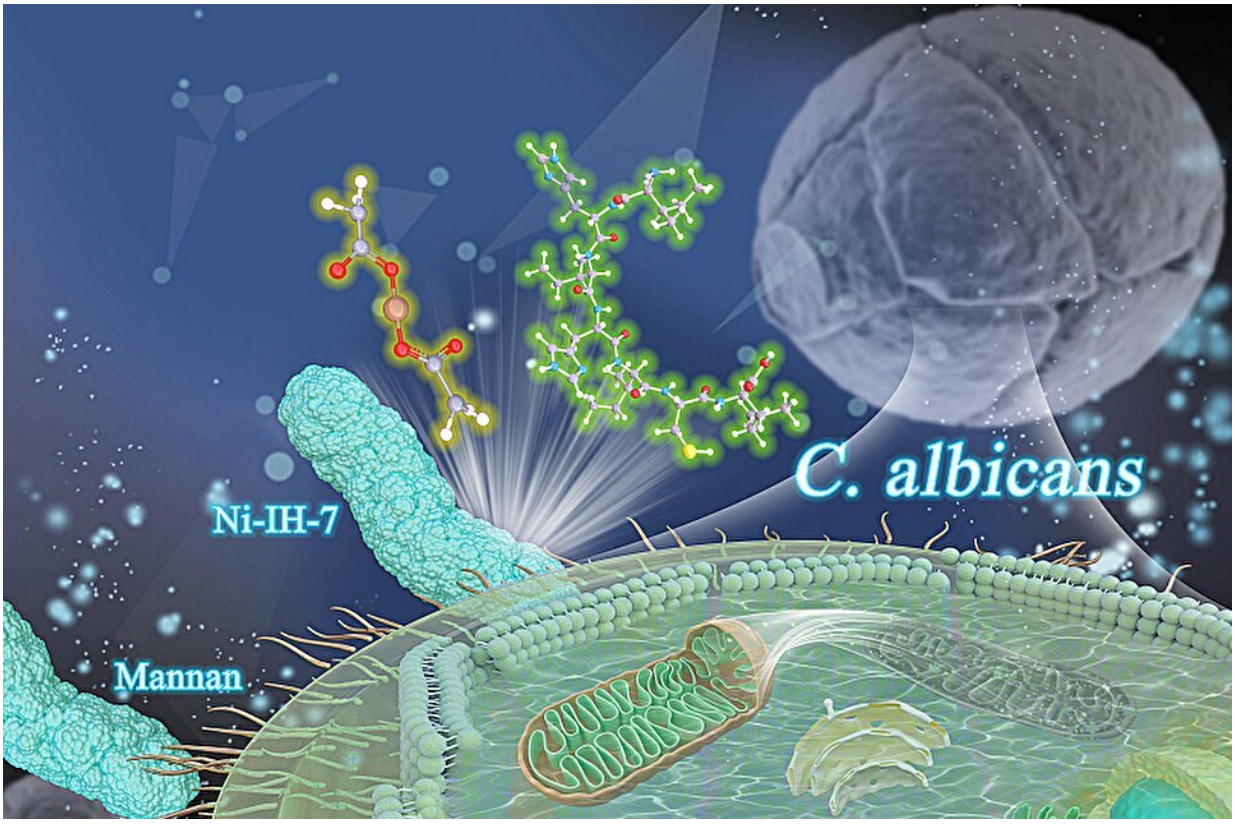
# Scientists develop dual-functional, high-efficiency antimicrobial nanozyme

July 17 2024, by Zhang Nannan




Antibacterial mechanism of Ni-IH-7 peptide nanozyme. Credit: Gao Lizeng's group

A research team led by Prof. Gao Lizeng from the Institute of Biophysics of the Chinese Academy of Sciences proposed a bactericidal

mechanism based on nanozymes that simulate antimicrobial peptides (AMPs) and antimicrobial enzymes (AMEs) according to biomimicry principles, and designed a dual-functional high-efficiency antimicrobial nanozyme.

Their research was published in *Nature Communications* on July 5.

Starting from the rational design of multi-peptide nanozymes, based on the key amino acids in the active sites of AMPs and AMEs, including histidine and cysteine, and combining peptide self-assembly and metal coordination principles, using various computational methods such as Alphafold2, molecular dynamics simulation, and density functional theory, the researchers optimized and selected a group of 7-peptide sequences IHIHICI.

The self-assembled nanozyme (AMPANs) possesses both AMP and AME functions, demonstrating specific and efficient fungicidal effects.

The researchers selected $Ni(Ac)_2$-assembled peptide nanotubes (Ni-IH-7) as the research object. Enzymatic studies showed that Ni-IH-7 has phospholipase C-like activity and peroxidase-like activity.

Due to the formation of a stable secondary structure nanotube, the Ni-IH-7 peptide nanozyme exhibited good tolerance to various hydrolytic enzymes.

In addition, they found that the Ni-IH-7 peptide nanozyme could selectively bind to the mannoprotein on the surface of Candida albicans and induce lipid peroxidation, leading to iron death and hydrolysis of glycerophospholipids, thus rapidly killing the fungi.

In vitro colony smear plate experiments on vaginal discharge from patients with vaginitis confirmed that the Ni-IH-7 peptide nanozyme had

good antifungal effects and the bactericidal performance was not compromised by other substances in the secretions.

This study is the first to propose the strategy of combining antimicrobial peptides with nanozymes, designing and synthesizing peptide nanozymes from scratch through computer simulation, and systematically studying their specific mechanism of killing fungi, providing insights for the development of novel antimicrobial drugs.

**More information:** Ye Yuan et al, Stable peptide-assembled nanozyme mimicking dual antifungal actions, *Nature Communications* (2024). DOI: 10.1038/s41467-024-50094-6

Provided by Chinese Academy of Sciences