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IISc develops computational models to speed up screening of antimicrobials

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Breaking down bacterial barriers with supercomputing

In two recent studies, researchers at the Indian Institute of Science (IISc), Bengaluru and Unilever have collaborated to develop computational models of bacterial cell walls that can speed up the screening of antimicrobials, molecules which can kill disease-causing bacteria.

Antimicrobials kill bacteria either by disrupting the cell wall's lipid membrane and destabilising the peptidoglycan layer, or by translocating through the cell wall layers and disrupting the cell membrane inside. However, the actual mechanisms of interaction between antimicrobial molecules and these cellular barriers are poorly understood.

The research team at IISc is the first to propose a comprehensive molecular model of the cell wall for Staphylococcus aureus. In one study, the team created an 'atomistic model', a computer simulation that recreates the structure of the cell wall down to the level of individual atoms. In the other study, the team used their model to compare the movement of different surfactant molecules through the peptidoglycan layer in E. coli.

Using the supercomputing facility at IISc, the team tested the effectiveness of their model with several known antimicrobials. One of these, melittin, a short peptide, binds with higher efficiency to the E. coli cell wall than that of S. aureus.

"The goal with Unilever is to facilitate rapid screening of molecules using the computational models we have developed, to narrow down the search for potential antimicrobials to a smaller subset of molecules which can be tested in the laboratory," said the researchers.