Computational cells to speed up screening of antimicrobials

January 14, 2023

In news– In two recent studies, researchers at the Indian Institute of Science (IISc) and Unilever have collaborated to develop **computational models of bacterial cell walls that can speed up the screening of antimicrobials.**

Key highlights-

- According to IISc, each bacterial cell is enveloped by a cell membrane, which is in turn surrounded by a cell wall.
- Some bacteria like Escherichia coli (E. coli) are Gram-negative, their cell walls contain a layer of peptide-sugar complexes called peptidoglycans and an outer lipid membrane.
- Others such as Staphylococcus aureus (S. aureus) are Gram-positive; their cell walls only have several layers of peptidoglycans.
- 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.
    - Antimicrobials are molecules which can kill disease-causing bacteria.
- 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.**
- They incorporated parameters such as the sizes of sugar chains in the peptidoglycans, the orientation of peptides, and the distribution of void size.

- In the other study, the teams used their **model to compare the movement of different surfactant molecules through the peptidoglycan layer in E. coli.**
- **Like detergents, surfactants have a water-loving head attached to a water-avoiding tail chain. The team showed for the first time the link between the length of the tail and antimicrobial efficacy of surfactants.**
- Surfactants like laurate with shorter chains translocated more efficiently than longer chain oleate.
- This was corroborated by experiments carried out by scientists in the Unilever team, which showed that shorter chain surfactants killed bacteria at a higher rate than surfactants with longer chains.