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Molecular Digital Twins of Innate Immunity: Insights from Simulations of Human Guanylate-Binding Protein 1

Wednesday, 4 March 2026 17:50 (20 minutes)

This work explores digital twins for innate immunity, focusing on human guanylate-binding protein 1 (hGBP1) and its role in targeting intracellular pathogens. Using coarse-grained molecular dynamics simulations, we examine protein-membrane interfaces with realistic pathogen membranes. We find that hGBP1 interacts with various membrane types; negatively charged lipids enhance affinity, while lipopolysaccharides are crucial for effective interactions. Additionally, hGBP1 polymerization is essential for stable membrane binding required for pathogen clearance.

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Session Classification: Short Talk