**INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI**
**SHORT ABSTRACT OF THESIS**

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Thesis Title: Computational Investigation of Cyclic Peptide Nanotubes: Self-Assembly, Solvent Effects, and Transport Behavior of Water and Ions

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**SHORT ABSTRACT**

The present thesis entitled “Computational Investigation of Cyclic Peptide Nanotubes: Self-Assembly, Solvent Effects, and Transport Behavior of Water and Ions” presents a comprehensive molecular dynamics investigation of cyclic peptide nanotubes (CPNTs), focusing on their self-assembly, stability, and transport properties across diverse environments. The self-assembly mechanism of cyclic peptides in aqueous solutions is examined, revealing salting-in and salting-out effects governed by NaCl concentration and enhanced nanotube formation at lower temperatures. The influence of solvent polarity and amino acid composition is then explored, demonstrating that non-polar solvents and alternating hydrophilic-hydrophobic residues stabilize the CPNT structure. Extending to deep eutectic solvents (DESs), simulations show that DESs markedly stabilize CPNTs, with stability diminishing upon increased hydration and temperature. Subsequent studies in lipid bilayers establish that CPNTs integrate seamlessly as synthetic water channels, maintaining characteristic water transport dynamics. Finally, ion transport studies reveal a strong preference for cations, particularly $Na^+$ and $K^+$, while anions face significant energy barriers. Together, these findings provide fundamental insights into CPNT behavior across environments and suggest their potential for applications in nanofluidic and biomimetic membrane systems.