Structural Ensemble of Peptide-induced Membrane Poration by Heterogeneous Magainin Peptides

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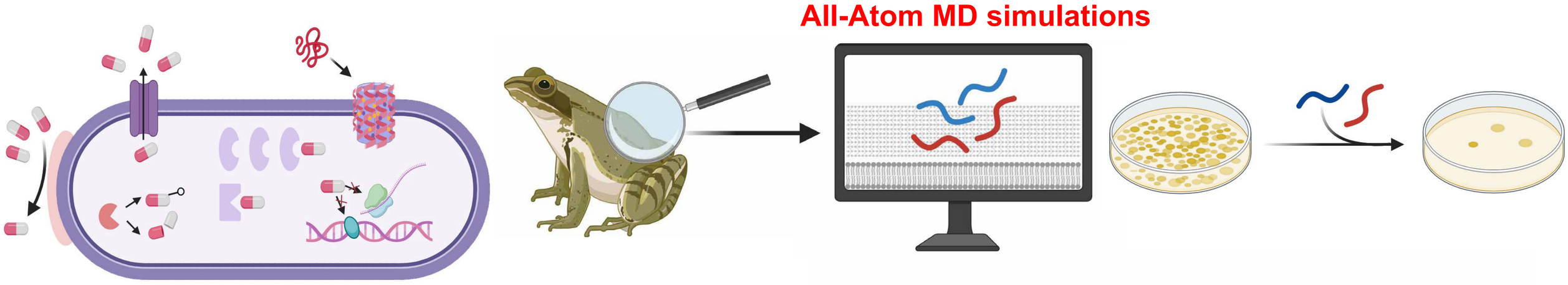
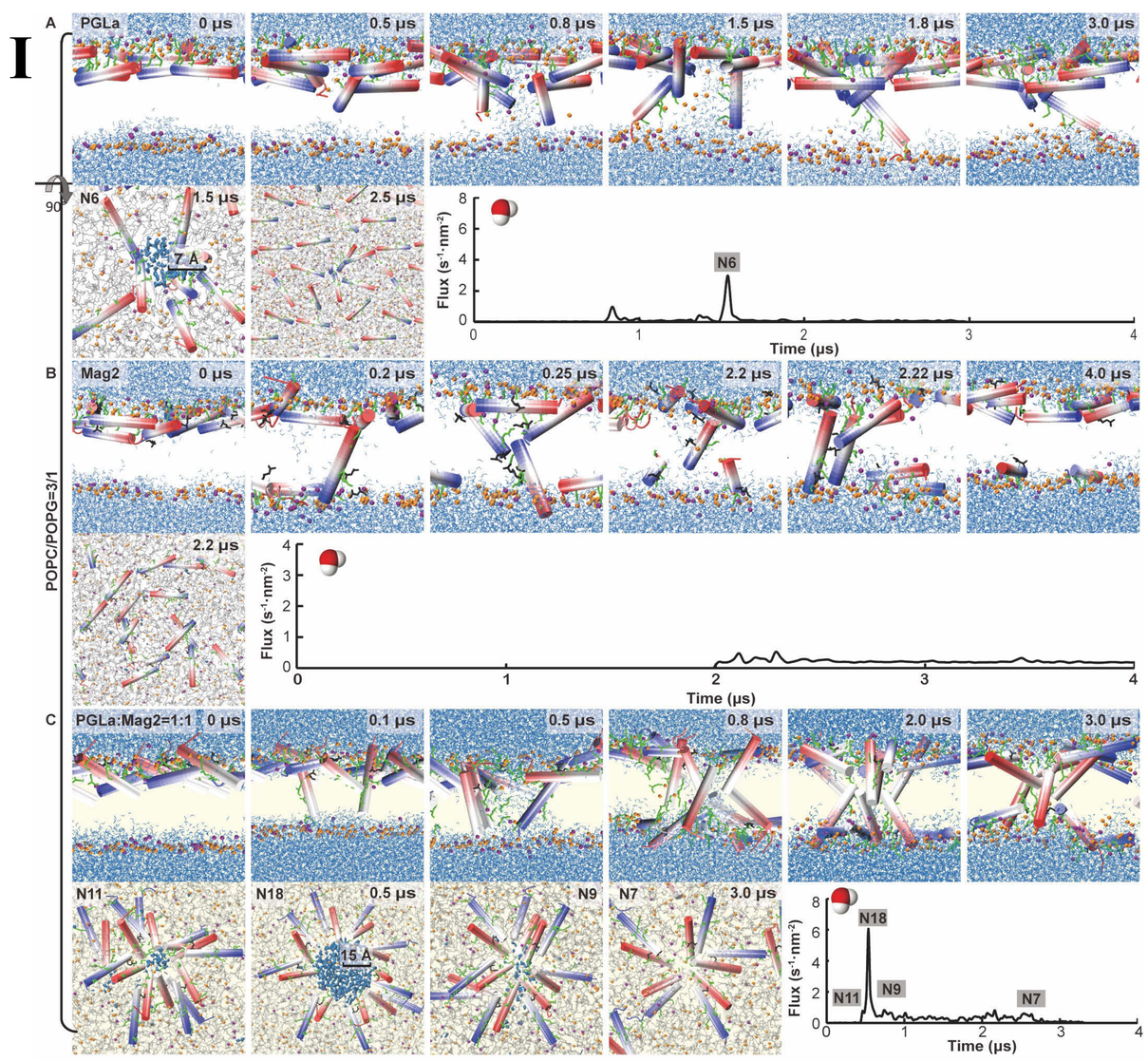
Introduction

Antimicrobial resistance has emerged as a significant global public health concern. Antimicrobial peptides (AMPs) hold potential as alternative therapeutic agents. However, a primary obstacle resides in the absence of effective experimental methodologies capable of investigating transient behaviors at the atomic scale.



Result1: Ab-initial microsecond-scale all-atom folding-assembly simulations can capture the spontaneous behavior of AMPs exhibiting membrane-disrupting activity.



Result2: Dynamic ensemble of pore architectures may explain the low potential of resistance development of AMPs.