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Simulation of Nucleic Acid Transport Through Carbon Nanotube Membranes[1]

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We use molecular dynamics simulations to study the electrophoretic transport of single-stranded ribonucleic acid (RNA) molecules through 1.5-nm wide pores of carbon nanotube membranes. During a total simulation time of ∼800 ns, we observe ∼170 individual RNA translocation events at full atomic resolution of solvent, membrane, and RNA. By analyzing structure, thermodynamics, and kinetics, we identify key factors for the membrane transport of biopolymers. We find that RNA entry into the nanotube pores is controlled by conformational dynamics. Exit from the pores is strongly affected by hydrophobic attachment of RNA bases to the pore walls. Translocations with and without such hydrophobic binding result in slow and fast exit from the pores. We use a trap-diffusion model to describe the pore-blockage statistics obtained from the simulations and earlier experiments using an alpha-hemolysin pore. The rate of hydrophobic trapping depends only weakly on the applied electric field, whereas the rate of dissociation from the pore walls increases exponentially with the field. In the absence of an external electric field, RNA remains hydrophobically trapped in the membrane despite large entropic and energetic penalties for confining charged polymers inside nonpolar pores. We find that differences in RNA conformational flexibility and hydrophobicity result in sequence-dependent rates of translocation, a prerequisite for nanoscale separation devices.

[1]with In-Chul Yeh