Different Hydration Patterns in the Pores of AmtB and RhCG Could Determine Their Transport Mechanisms

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The ammonium transporters of the Amt/Rh family facilitate the diffusion of ammonium across cellular membranes. Functional data suggest that Amt proteins, notably found in plants, transport the ammonium ion (NH4(+)), whereas human Rhesus (Rh) proteins transport ammonia (NH3). Comparison between the X-ray structures of the prokaryotic AmtB, assumed to be representative of Amt proteins, and the human RhCG reveals important differences at the level of their pore. Despite these important functional and structural differences between Amt and Rh proteins, studies of the AmtB transporter have led to the suggestion that proteins of both subfamilies work according to the same mechanism and transport ammonia. We performed molecular dynamics simulations of the AmtB and RhCG proteins under different water and ammonia occupancy states of their pore. Free energy calculations suggest that the probability of finding NH3 molecules in the pore of AmtB is negligible in comparison to finding water. The presence of water in the pore of AmtB could support the transport of proton. The pore lumen of RhCG is found to be more hydrophobic due to the presence of a phenylalanine conserved among Rh proteins. Simulations of RhCG also reveal that the signature histidine dyad is occasionally exposed to the extracellular bulk, which is never observed in AmtB. These different hydration patterns are consistent with the idea that Amt and Rh proteins are not functionally equivalent and that permeation takes place according to two distinct mechanisms.

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