Ammonium Transporters Achieve Charge Transfer by Fragmenting Their Substrate

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Proteins of the Amt/MEP family facilitate ammonium transport across the membranes of plants, fungi, and bacteria, and are essential for growth in nitrogen-poor environments. Some are known to facilitate the diffusion of the neutral NH3 while others, notably in plants, transport the positively charged NH4+. Based on the structural data for AmtB from Escherichia coli, we illustrate the mechanism by which proteins from the Amt family can sustain electrogenic transport. Free energy calculations show that NH4+ is stable in the AmtB pore, reaching a binding site from which it can spontaneously transfer a proton to a pore-lining histidine residue (His168). The substrate diffuses down the pore in the form of NH3 while the excess proton is co-transported through a highly conserved hydrogen-bonded His168-His318 pair. This constitutes a novel permeation mechanism that confers to the histidine dyad an essential mechanistic role that was so far unknown.

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