A stable water chain in the hydrophobic pore of the AmtB ammonium transporter

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The accessibility of water molecules to the pore of the AmtB ammonium transporter is studied using molecular dynamics simulations. Free energy calculations show that the so-called hydrophobic pore can stabilize a chain of water molecules in a well of a few kcal/mol, using a favorable electrostatic binding pocket as an anchoring point. Moreover, the structure of the water chain matches precisely the electronic density maxima observed in x-ray diffraction experiments. This result questions the general assumption that the AmtB pore only contains ammonia (NH(3)) molecules diffusing in a single file fashion. The probable presence of water molecules in the pore would influence the relative stability of NH(3) and NH(4)(+), and thus calls for a reassessment of the overall permeation mechanism in ammonium transporters.

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