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Free Energy Wells and Barriers to Ion Transport Across Membranes¹

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The flow of ions across cellular membranes is essential to many biological processes. Ion transport is also important in synthetic materials used as battery electrolytes. Transport often involves specific ions and fast conduction. To achieve those properties, ion conduction pathways must solvate specific ions by just the “right amount.” The right amount of solvation avoids ion traps due to deep free energy wells, and avoids ion block due to high free energy barriers. Ion channel proteins in cellular membranes demonstrate this subtle balance in solvation of specific ions. Using ab initio molecular simulations, we have interrogated the link between binding site structure and ion solvation free energies in biological ion binding sites. Our results emphasize the surprisingly important role of the environment that surrounds ion-binding sites for fast transport of specific ions.

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