The molecular dynamics of potassium channel permeation, selectivity and gating

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Ion channels facilitate the passive, selective permeation of ions such as sodium, potassium and chloride across biological membranes and as such are essential for cellular electrical signalling. Molecular dynamics simulations are used to study ion permeation across potassium channels at the atomic level. Together with crystallographic analyses and electrophysiological experiments these provide insight into the mechanisms of selective and efficient permeation of potassium, as well as the complex and subtle conformational changes involved in the gating of these channels.