

# **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 signaling. Molecular dynamics simulations based on the computational electrophysiology scheme will be presented to study ion permeation across potassium channels. Together with crystallographic analyses and electrophysiology experiments these provide insight into the mechanisms of permeation, selectivity and gating in potassium channels.