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On the activation and modulation of voltage gated ion channels

Excitable cells produce electrochemical impulses mediated by the transport of ions across their membrane through voltage gated ion channels (VGCs). In this talk, we show that the atomistic description of VGC activation obtained by molecular dynamics simulations and free energy calculations is consistent with the phenomenological models adopted so far to account for the macroscopic currents measured by electrophysiology. These results pave the way for a deeper understanding of the molecular level factors affecting ion channel activation such as lipid composition, amino acid mutations, and binding of drug molecules or endogenous ligands.

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