# How Do Calcium Ions Permeate through the Ryanodine Receptor 1

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**Abstract:** The ion permeation mechanisms of channel proteins have been widely studied with molecular dynamics (MD) simulations. However, it has been a challenge for $Ca^{2+}$ channels due to the absence of a reliable ion model that can reproduce the interaction between $Ca^{2+}$ and biomolecules quantitatively. I will present a recently developed multi-site $Ca^{2+}$ model in the framework of classical MD simulations, which showed a high accuracy describing the interaction energies between ions and proteins. With this model, we were able to reveal the atomistic details of $Ca^{2+}$ permeation through the ryanodine receptor 1, an essential channel protein responsible for the precise control of the cytosolic $Ca^{2+}$ concentration and muscle contraction. Our results showed that the $Ca^{2+}$ permeation process through the ryanodine receptor 1 is distinct from the widely studied ion permeation mechanisms of $K^+$ and $Na^+$ channels, thus shedding lights on the underlying reasons for the high permeability and week selectivity of the ryanodine receptors.