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Presentation Abstract

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Abstract Title:	MONTE CARLO SIMULATION OF FREE ENERGY COMPONENTS: ENERGETICS OF SELECTIVE BINDING IN A REDUCED MODEL OF L-TYPE CA CHANNELS

Author Block: **Janhavi Giri**[1,2], Bob Eisenberg[2], Dirk Gillespie[2], Douglas Henderson[3], Dezső Boda[4].
[1]University of Illinois at Chicago, Chicago, IL, USA, [2]Rush University Medical Center, Chicago, IL, USA, [3]Brigham Young University, Provo, UT, USA, [4]University of Pannonia, Veszprém, Hungary.

Abstract Body: A reduced model of voltage-gated L-type Ca channels is used to study the energetics of selective binding of Ca^{2+} versus monovalent and divalent cations. Widom's particle insertion method is combined with Grand Canonical Monte Carlo simulations to compute the electrostatic and excluded volume components of the free energy difference between channel and bath. We have shown (in ~ 30 papers) that selectivity of the L-type Ca channel and voltage activated Na channel can both be described (over a wide range of solutions and concentrations) by the same reduced model with the same unchanging two parameters (dielectric coefficient and diameter) in which side chains are spheres (Ca channel = EEEE or EEEA; Na channel = DEKA). In the EEEE channel, Ca^{2+} selectivity is driven by charge/space competition in which selectivity arises from a balance of electrostatics and the excluded volume of ions in the crowded selectivity filter. Electrostatics selects Ca^{2+} over monovalent cations. Excluded volume selects Ca^{2+} over larger divalent cations. All these combine to

create depletion zones in the ionic density profiles that are crucial determinants of the current carried by each ionic species.

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Biophysical Society
9650 Rockville Pike
Bethesda, MD 20814
Phone: 301.634.7114