Seminar Series of the
CIHR Training Grant in

Protein Folding and Interaction Dynamics

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Voltage-gated potassium ion channels are frustrated: insights into protein dynamics from molecular dynamics simulations

Voltage-gated potassium (Kv) channels open or close in response to changes in the transmembrane (TM) potential. Structures of several open mammalian Kv channels are known and a hypothesis for how they close has been proposed. There is, however, no general hypothesis explaining how they open. Here we show that the Kv1.2/2.1 chimaera becomes strained when closed. Our free energy molecular dynamics simulations suggest that the pore-lining (S6) helices prefer to remain kinked. When the TM potential becomes negative, the voltage sensors move down and do work on the S6 helices, straightening them, and closing the pore. Upon depolarisation, the voltage sensors move back up and the S6 helices therefore spring open and relieve the strain.

Host: Dr. Reinhart Reithmeier

Thursday, May 1, 2014 - 12:00pm
Medical Sciences Building, Rm. 4279
University of Toronto