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Computational Simulations of Asymmetric Fluxes of Large Molecules Through Gap Junction Channel Pores

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Abstract.

Gap junction channels are formed of connexin isoforms, which enable molecule and ion selective diffusion amongst neighboring cells. HeLa cells expressing distinct connexins (Cx) allow the formation of heterotypic channels, where we observed a molecular charge-independent preferential flux of large fluorescent molecules in the Cx45 to Cx43 direction. We hypothesize that the pore's shape is a significant factor along-side charge and transjunctional voltages for this asymmetric flux. To test this hypothesis, we developed a 3D computational model simulating Brownian diffusion of large molecules in a gap junction channel pore. The basic pore contour

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