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## Elucidating proton-mediated conformational changes in the acid-sensing ion channel 1a through molecular dynamics simulation

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Acid-sensing ion channel 1a (ASIC1a) as proton-activated receptor cation channel, contributes to sensory transduction, depression and fear-related behaviors throughout nervous system. So far, how proton mediates the channel gating process still remains elusive. Here we report that the ion pore changes at different PH values through molecular dynamics (MD) simulations. The path of long-range conformational changes from the extracellular domain to the transmembrane domain was determined; further, the correlation network analysis reveals how the interactions between subunits influence the channel gating changes.  $\beta 1$ ,  $\beta 2$ ,  $\beta 10$ ,  $\alpha 6$ ,  $\alpha 7$ ,  $\beta 11$  and  $\beta 12$  are the crucial regions by forming a passageway to regulate the ion pore changes. Our results reveal the process that the extracellular domain remotely regulates the pore changes.

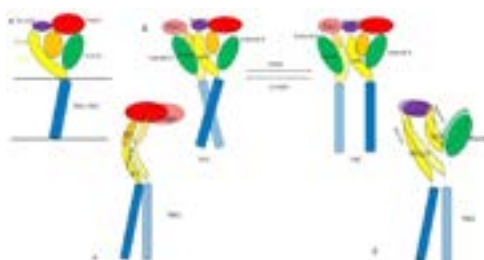


Figure 1: Schematic representation of the ASIC1a ion channel structure. The diagram shows the channel composed of two subunits, each with an extracellular domain (top) and a transmembrane domain (bottom). The extracellular domain is shown in various colors (red, yellow, green, blue) representing different regions. The transmembrane domain is shown in blue. The channel is shown in a closed state (left) and an open state (right), with arrows indicating the direction of conformational change. The ion pore is shown in the center of the transmembrane domain.

### Biography

Xu-ri Huang has completed his PhD in 1991 from Jilin University. Now He is a professor of Institute of Theoretical Chemistry, Jilin University. His research focuses on theoretical chemistry, such as catalysis reaction mechanism and biomolecular simulation. He has published more than 150 papers in reputed journals.

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