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Regulating the Acid-sensing ion channel1a with Psalmotoxin1 through molecular dynamics simulation

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Acid-sensing ion channel 1a(ASIC1a) is a cation channel activated by protons and causes Nerve death through central nervous system. Psalmotoxin1 is a gating modifier for ASIC1a. How the PcTx1 in complex with ASIC1a regulates the channel gating from the extracellular domain to the transmembrane domain is unclear. Here we used molecular dynamics (MD) simulations method to report the function of residues on PcTx1 and the path to change the ion pore. $\beta 1$, $\beta 2$, $\beta 10$, $\alpha 6$, $\alpha 7$, $\beta 11$ and $\beta 12$ provide crucial the passageway to influence to channel gating through analyzing the PCA results and residues Arg27 is the main reason to stabilize the open state of the pore through researching the hydrogen bonds, combining with the correlation network analysis.

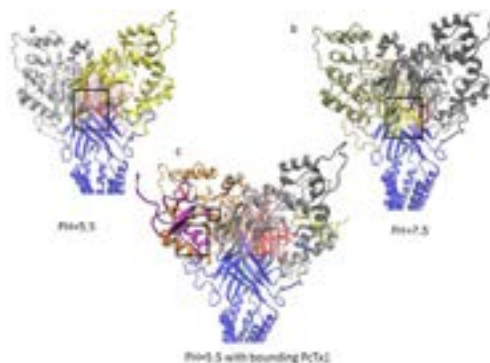


Figure1. Community partitioning from correlation network analysis reveals differences at P415.5 with bounding the PcTx1 . P415.5 and P417.5, respectively. The view of structure is: interface between subunit A and subunit C, which is perpendicular to the film to the membrane. The black frames mark the single community.

Biography

Xi Zhao obtained his PhD in 2007 from Jilin University and was a visiting scholar from Department of Chemistry at University of California, Irvine. Now he is an associate professor of Institute of Theoretical Chemistry, Jilin University. His researches focus on biomolecular simulation. He has published more than 30 papers in reputed journals.

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