Title: Molecular dynamics simulations of ion channel TRPA1

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Abstract: The ion channel TRPA1 is one of the members of the transient receptor potential channel family. These channels have recently been an important objective of research, because they play important roles in various cellular processes and organismic mechanisms. Especially they are involved in most of the senses. We focused mainly on the TRPA1 ion channel due to its involvement in the pain sensation in humans. Because the molecular mechanisms behind the gating of this channel are not fully understood, their description is a key for a design of new analgesics targeting this channel. We used a homology modeling and molecular dynamics simulations in conjunction with electrophysiological experiments to provide a valuable new insight into the channel mechanisms. We contributed by describing of a putative binding site for calcium ions. Further, many functionally important amino acids were found in the S1–S4 transmembrane domain.

Keywords: voltage-gated ion channel, TRPA1 channel, molecular dynamics, homology modeling