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Abstract

In silico Analysis of Structure Activity Relationship of ω-Conotoxins with Cav 2.2 Channel Receptor for Treatment of Neuropathic Pain

Muhammad Sibte Hasan Mahmood
MBBS, Rawalpindi Medical College in Pakistan, Canada

Abstract:

The N-type voltage-gated Ca2+ channel Cav2.2 is expressed predominantly at presynaptic neuronal terminals. They are predominantly expressed in nerve terminals, where they control neurotransmitter release. Also, this receptor transduces electrical activity into other cellular functions and plays an important role in processing pain information in nociceptive pathways. To date, genetic and pharmacological studies have identified that high threshold, Cav 2.2 channel receptor is important for pain sensation in disease models. This suggests that Cav 2.2 channel receptor inhibitors or modulators could be developed into useful drugs to treat neuropathic pain. Thus, they are molecular targets for pharmacological agents as well as for broad range of potent neurotoxins. Cav 2.2 channels are reported as main target of ω-conotoxins

Many peptides are reported as potent and highly selective blockers of calcium channel function. Among them, cone snails are rich sources of such peptides and constitute class of conotoxins. In this study, structural and binding analysis of ω-conotoxins class have been done against Cav 2.2 channel receptor to investigate their role as therapeutic agents and analgesics. The, α1 subunit of Cav 2.2 channel receptor is essential for channel functioning and determines fundamental channel properties. Domain III region of α1 subunit of Cav 2.2 channel receptor is the molecular target for broad range of venom toxins. These toxins act on region between S5 and S6 helices of domain III. These toxins physically block the pore of receptor. The binding site of these toxins has been mapped primarily to the external vestibule of the channel in the domain III pore-forming S5-S6 region. In particular, the residues Glu1326, Gln1327, Glu1332, Glu1334, Glu1337 and Gln1339 were identified as being important for blockage by ω-conotoxins. As ω-conotoxins have surfaced their potential as modulators of Cav2.2 channel. So, in this study a data set of 16 different ω-conotoxins was taken to study binding interactions with the Cav 2.2 channel receptor computationally.

Biography:

Muhammad Sibte Hasan Mahmood received his MBBS degree from Rawalpindi Medical College in Pakistan. He has worked as a physician in Pakistan for various health care providers. Since moving to Canada in 2015, he has focused more attention to research and study trials. Working with renowned researchers in various medical fields either under direct or indirect supervisions has offered invaluable experience and learning. His main areas of focus have been drug mechanics and therapeutic modelling. He strives to achieve a long-lasting impact in the field of clinical and pharmacologic research and development.

Publication of speakers:

1. Kalsoom, Qudsia & Hasan, Sibte. (2019). Reflective Actions for Sustainable Development.
2. Aziz, Fakhra & Kalsoom, Qudsia & Quraishi, Uzma & Hasan, Sibte. (2017). Perceptions on gender-based differences in educational leadership. Management in Education. 31. 089202061769662. 10.1177/0892020617696628.
3. Kalsoom, Qudsia & Amin, Muhammad & Hasan, Sibte. (2016). Factors Directing Curriculum Debate among Teacher Educators in Pakistan. 132-146.

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