

Computational Approach to the Interaction of Neurotoxins and Kv1.3 Channel

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Abstract : Sea anemone neurotoxins are peptides that interact with Na⁺ and K⁺ channels, resulting in specific alterations on their functions. Some of these neurotoxins (1ROO, 1BGK, 2K9E, 1BEI) are important for the treatment of nearly eighty autoimmune disorders due to their specificity for Kv1.3 channel. The aim of this study was to identify the common residues among these neurotoxins by computational methods, and establish whether there is a pattern useful for the future generation of a treatment for autoimmune diseases. Our results showed eight new key common residues between the studied neurotoxins interacting with a histidine ring and the selectivity filter of the receptor, thus showing a possible pattern of interaction. This knowledge may serve as an input for the design of more promising drugs for autoimmune treatments.

Keywords : neurotoxins, potassium channel, Kv1.3, computational methods, autoimmune diseases

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