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Investigating the Binding Mechanism of hERG Potassium Channel using Scorpion and Sea Anemone Venoms as Therapeutic Agents

Tiyyaba Furqan
Comsats University Islamabad, Pakistan

Bioactive proteins and peptides from venom of different species have shown to possess potential for therapeutic uses in a number of diseases such as cancer, cardiovascular and neurological disorders as well as in metabolic and autoimmune diseases. Peptide toxins are used for prey acquisition, but also to deter potential predators and even to fight territorial disputes. Various peptide toxins separated from animals, attack for potassium channel inhibition with high affinity binding to different sites of KV11.1. Scorpion and Sea Anemone venom ligand residues interact at the different sites of voltage gated potassium channel inhibiting potassium channel by altering its function. The docking depicts the inhibitory potential of Scorpion and Sea Anemone venoms for the voltage gated potassium channel that provides therapeutic opportunity for treating several channelopathies like neurological disorders, cardiovascular disorders and metabolic disorders.the potassium ion (K+) channels, especially they play key role to inhibit the potassium voltage-gated channels K+ (KV). In this study, the BDS potassium channel toxin family from scorpion and gamma ktx family from sea anemone are used. The hERG channel is a voltage-gated potassium channel involved in cardiac action potential repolarization. The marginalized function of hERG extends ventricular action potentials, increase the QT interval in an electrocardiogram, and advances the risk for lethal ventricular arrhythmias. KV channels offer vast variety for development of new drugs for cancer, cardiovascular and neurological disorders, autoimmune and metabolic diseases.

This study focuses on the binding analysis of toxin ligands with human voltage-gated potassium channel receptor, through structural comparison, for their potential therapeutic use in treating several diseases. The ligands and the receptor dataset were retrieved for in silico analysis and docking experiments were performed to analyzed the binding interactions between them. The ligand dataset comprises of 31 proteins of Type 3 BDS toxin family form Sea Anemones and 11 proteins of Gamma ktx family from scorpions. The KV11.1 is used as receptor for identifying the interaction sites of the abovementioned ligands. Hex software is used to check each protein of BDS Type 3 Toxin Family and Gamma ktx, docked with receptor kv11.1, for identifying the residues involved in hydrogen bonding and hydrophobic interactions.

The analysis revealed that the protein venoms of sea anemone and scorpion have binding interactions with receptor binding sites. The structures of the BDS type 3 toxin family and Gamma ktx family are rich in dissulphide domain and the main protein venom residue Lysine (Lys 6, Lys 28, Lys 116 Lys 116 and Lys 101, was predominantly observed in binding interaction with KV11.1. The docking results revealed that Lysine is important for potassium channel inhibition with high affinity binding to different sites of KV11.1. Scorpion and Sea Anemone venom ligand residues interact at the different sites of voltage gated potassium channel

inhibiting potassium channel by altering its function. The docking depicts the inhibitory potential of Scorpion and Sea Anemone venoms for the voltage gated potassium channel that provides therapeutic opportunity for treating several channelopathies like neurological disorders, cardiovascular disorders and metabolic disorders.

Biography

Tiyyaba Furqan has completed her MS in Molecular Genetics from the Biosciences Department of Comsats University Islamabad, Pakistan during 2018-2020. After her graduation, she started working as a research assistant at the Biosciences lab under the supervision of Dr. Syed Muhammad Nurulain and Dr. Sidra Batool at Comsats University Islamabad, Pakistan. Her area of research includes the drug designing and development, computational analysis, neuroscience, and molecular genetics. For the past couple of years, she has been helping students in conducting their research and lab work, publishing their research, and focusing on skills acquisition. She has published a number of research articles as a first author as well as a coauthor in internationally recognized high impact factor journals. She has worked effectively and efficiently with international collaborators to complete her research studies. Her current research interests for PhD include pharmacology and pharmacogenomics for the treatment of various diseases.

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