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Molecular studies of scorpion toxins interactions with calcium-activated potassium channels

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The calcium-activated potassium channels (KCa channels) are widely expressed in the organism. Several studies demonstrated the potential role of KCa3.1 channel blockage as a therapeutic strategy. Knowledge of the molecular aspects of blockers binding process is an important step in designing highly efficient and selective ligands. Aim of this study was an interface analysis in complexes of hybrid channel KcsA-KCa3.1 with peptide blockers agitoxin, charybdotoxin and maurotoxin. KcsA-KCa3.1 chimera represents KcsA channel with P-loop taken from the human KCa3.1. 3D structure was generated by homology modeling using complex of mutated KcsA channel with charybdotoxin (pdb-code 2A9H) as a template. Molecular dynamic simulation was performed using Gromacs software. Optimal conformations of toxins in channel binding site were chosen from the trajectories. Hydrophobic and stacking interactions, hydrogen and ionic bonds of the toxins and hybrid channel were evaluated using program Platinum and APBS software package. Contacts energy characteristics evaluation showed that maurotoxin was the most effective blocker of KCa3.1 channel among these toxins. This result is in good agreement with the experimental data. Knowledge of channel-toxins interfaces allowed us to propose amino acid mutations in toxins to increase binding affinity and selectivity. Results of the conducted investigation are of great interest for drug development.

Biography

Alena Dmitrievna Volyntceva is a Post-graduate student of Chair of Bioengineering at the Faculty of Biology, Lomonosov Moscow State University. She is the Junior Reseacher and has been investigating receptor-ligand interactions for six years in the Laboratory of Molecular Dynamics and Molecular Modeling. Her current interests includes "Study of potassium channels interactions with scorpion toxins".

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