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Identification of hot-spot regions of N-type Ca^{2+} channel receptor by its homology model and molecular dynamics based blocker design

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Proteins are heterogeneous macromolecules, consisting of hundreds to several thousands of atoms. How a protein spontaneously forms a well-defined biologically active structure is a fascinating and still open question? However, solving the protein folding problem would also have great practical implications. Molecular dynamics simulations has been applied extensively nowadays for the refinement of structures derived from X-ray diffraction and NMR data, and for understanding the dynamic mechanism of the enzyme and its inhibitory action, to the study of protein structure prediction, study of biopolymer aggregates like membranes and structure-based drug design.

Molecular dynamics simulation study of the closed state of the NCC receptor at the pore forming domains (S5-P-S6) was performed for 50 ns simulations. The study revealed the structural stability and its dynamic behavior with respect to channel blockers. The present study is useful in understanding the NCC receptor atomic level dynamic interactions with its blocker (antagonist), which will in turn guide in designing potent and effective NCC receptor blockers. Further study of the open state of the NCC receptor at the pore forming domains (S5-P-S6) was also presented to address the dynamic mode of opening and closing of this receptor.

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