Molecular Dynamics Simulation Study of Brazilian Frog Dermadistinctin K Peptide in TFE/water Mixture Environment.

Batista, M. M\textsuperscript{1,2}; Fernandes, T. V. A.\textsuperscript{2}; Santoro, M. M. Santoro\textsuperscript{1}; Pascutti, P. G.\textsuperscript{2}.

\textsuperscript{1} Departamento de Bioquímica e Imunologia, Universidade Federal de Minas Gerais, Minas Gerais, Brazil \textsuperscript{2} Laboratório de Modelagem e Dinâmica Molecular, Instituto de Biofísica Carlos Chagas Filho, Universidade Federal do Rio de Janeiro. Rio de Janeiro-RJ, Brazil.

Modern science is looking for new antimicrobial compounds to avoid persistent infections, because classical chemotherapies have been ineffective on those infections. Natural substances from animal toxins are the new focus of study as potential antimicrobial peptides. \textit{Phylomedusa distincta} is a Brazilian frog that has on the skin dermaseptins like Dermadistinctin K (DDK). DDK is an \(\alpha\)-helical peptide that attacks the bacteria biomembrane instead human cell membrane. The knowledge of peptide action mechanism is important to design new generation of antibiotics. Since DDK function is well established, computer simulations are showing how peptide works on different environment, that is important to control and improve its action. In this study we have simulated DDK in TFE/water mixture and in water. The structural and dynamical properties of DDK were compared to NMR data. Molecular Dynamics in TFE/water mixture aided to keep the stability of DDK \(\alpha\)-helix and provided a better understanding of conformational changes that allowed the peptide stabilization through biomembranes. TFE/water environment is important to simulate the membrane/water interface, and separate the hydrophilic and lipophilic side-chain of the peptide.

Word Keys: TFE-water mixture, molecular dynamics, dermaseptins, Dermadisctinctin, \(\alpha\)-helix stability, \textit{Phyllomedusa distincta}.

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