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Title (English)

# Molecular dynamics simulations; comparisons of octameric and tetrameric channel models of the peptaibol antiamoebin

Title (Swedish)

Abstract

Two different models of the channel bundle of the peptaibol antiamoebin were studied using molecular dynamics simulations in an explicitly modeled environment consisting of a POPC bilayer surrounded by water. Both the octameric and tetrameric bundles were found to be stable over tenths of nanoseconds with characteristic interhelical hydrogen bonding patterns stabilizing the channels. The dimensions of the channels have also been assessed and compared to each other and the modern potassium channels.

Keywords

antiamoebin, molecular dynamics, channel modeling, ion channels, protobiotic evolution

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