Influence of the Length in Biomimetic Ion Channels Based on Derivatized α,γ-Self Assembled Peptide Nanotubes. A Molecular Dynamics study.

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Abstract. We present here a Molecular Dynamics study on internally functionalized peptide nanotubes composed of cyclic peptides formed by α and γ-amino acids self-assembled in lipid bilayers. One of the main advantages of this type of nanotubes is that they have a partially hydrophobic inner cavity that can be easily derivatized using different functional groups. In this work we study the influence of the number of cyclic peptides, with four hydroxyl groups in their lumen, on the transport capabilities of the channels formed across the membrane. Using Molecular Dynamics simulations we studied how the length of the inner functionalized nanotubes affects to the transmembrane transport of different ions and to the structural and dynamical behaviour of both the modified peptide nanotubes and the DOPC membrane where they are inserted.