

TSX as a nucleoside channel

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E. coli TSX channel is a bacterial outer membrane channel that shows a strong substrate specificity for nucleosides. Beyond this role it is also suspected to be a channel for antibiotics entry into the bacterial interior and as a receptor for colicin K. In 2004, three crystallographic structures for TSX were published by Ye et al. Two of these structures were crystallized with ribonucleoside uracil and deoxyribonucleoside thymine. The residues were found bound in two distinct configurations at two binding sites. We use these structures as the starting points to study the nature of interactions of the channel with the nucleosides using molecular dynamics simulations and to understand what confers them specificity for the nucleoside substrates. Additionally, we calculate the relative free energy of binding for these sites and the free energy barriers within the TSX channel from Umbrella Sampling simulations. Using applied electric field simulations, we also calculate the ionic conductivity of the channel. In order to establish how the dynamics of the channel affects the conduction of the nucleosides, we present the ellipsis tool that calculates the area of the protein interior along the channel coordinate.

References

1. F. Author, Journal **volume**, page (year)