

Diffusion coefficients of antibiotics in aqueous ionic solutions

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Diffusion process is one of the main mechanisms of the delivery of antimicrobials to bacteria. The diffusion coefficients, together with their free energy profiles along the path, are necessary quantities in order to describe and understand the translocation kinetics of molecules through porins.

In this work, we present a database of the calculated translational and rotational diffusion coefficients of a set of known antibiotics of different families in the aqueous ionic solution. We study the dependence of the calculated diffusion coefficients on the charge state of the molecule. By modeling the molecules as ellipsoids, we show how their asymmetry affects the mobility. We discuss a generalized Stokes model relating the diffusion coefficients to the size and the shape of the molecule, and to the viscosity of the medium. We also show how the diffusion coefficient of a molecule changes in the confined space with respect to bulk conditions due to hydrodynamic effects.