

Translocation of phosphonic acid antibiotics through OmpF

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OmpF (Outer membrane Protein F) is a non-specific porin located in the outer membrane of the Gram-negative *E. Coli* bacterium . This porin is responsible for the translocation of many antibiotics and other hydrophilic substrates with molecular weights less than 600 Da. Phosphonic acid containing antibiotics like fosfomycin and fosmidomycine are used in the treatment of Gram-negative bacterial diseases and these drugs function by inactivating the enzymes MurA and Dxr, respectively, which in turn inhibit the bacterial cell growth. The pre-requisite for these antibiotics to function effectively is their need to pass through the bacterial outer membrane and it is very important to understand the translocation for these antibiotics for the design and development of drugs with improved permeability. In the present study, we employed applied field MD simulations on OmpF-fosfomycin and fosmidomycine systems to gain a molecular level insight into the translocation events of these phosphonic acid containing antibiotics.