Exploiting the OprE porin pathway in *Pseudomonas aeruginosa*. How to get large drugs through small pores?

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The main focus of our study is to identify the structural features responsible for the transport of molecules through substrate-specific channel OprE of Gram negative bacterium *Pseudomonas aeruginosa*. We present a precise molecular analysis of the structure and dynamics of OprE to explain the translocation of natural amino acid residues and antibiotics of two different chemical families through it. We used molecular dynamics simulations to obtain information on the molecule-channel interactions and proposed quantitative structure–function relationships based on them. We found some physical and chemical properties of the molecules playing an important role in modulating the translocation through OprE. Molecules with zwitterionic structures have an affinity towards the polar eyelet region and the presence of negative charge helps interaction with the basic ladder facilitating translocation. A favorable chemical structure helps to widen the otherwise small constriction region aiding translocation of relatively large antibiotics.