Molecular basis of selectivity and permeation in OpdH channel

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The members of outer membrane carboxylate channels (Occ) family facilitate the uptake of a wide range of small carboxylic compunds into the bacterial cell [1]. Despite extensive structural and functional studies [2], atomic-level mechanistic details of such transport process, and as importantly, their preference for specific molecules, has remained elusive. Here, we present energetics and transport pathways of ions, substrates and antibiotics through OpdH/OccK5, a member of Occ family, using all-atom molecular dynamics (MD) simulations. Furthermore, we show specific molecular interactions between channel and permeant molecules which facilitate its passage through the channel.

References

[1] S. Tamber et al., J. Bacteriol. **188**, 45-54 (2006)

[2] E. Eren et al., J. Biol. Chem. **288**, 12042-12053 (2013)