Simulations of OmpE36 porin in different memebrane models

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The interactions between lipopolysaccharides (LPS) and proteins play a pivotal role in providing a stable and impermeable outer membrane for Gram-negative bacteria [1, 2]. A X-ray crystallographic study of the OmpE36 porin from *Enterobacter Cloacae*, revealed details of the interactions at an atomic level by providing high-resolution structures of porins with bound rough LPS. However, it remained unclear about how the LPS influences the structure and dynamics of the pore. We addressed these questions by means of a series of long molecular dynamics simulations. Our study confirmed the LPS binding sites observed in the crystal packing and support them as biologically relevant lipid positions. Furthermore, the role of electrostatic interactions in mediating a tight interaction between the LPS and the pore is detailed. Moreover, our simulations along with the recent X-ray crystallographic results provide a full picture of molecular details concerning the functional interactions that impact the dynamics of the pore.

References

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