

## ***In silico* study of specific porins from *Acinetobacter baumannii***

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*Acinetobacter baumannii* is a Gram-negative bacterium considered one of the most dangerous pathogen due to its high resistance to practically all available antibiotics. As in *Pseudomonas Aeruginosa*, the outer membrane does not possess large general channels. In this study we are interested in understanding the mechanism of substrates transport as well the translocation of some b-lactam antibiotics through five specific porins from *A.baumannii*, recently crystallized and solved at high resolution. For that purpose, we performed a structural analysis comparing the results with data obtained for the homologous OccD and OccK porins from *P.aeruginosa*. Secondly, we used molecular dynamics simulations with enhanced sampling techniques to understand the mechanisms of small molecule permeation. These studies will help our understanding of (i) the structural and functional characteristics of these specific porins in filtering natural substrates and (ii) how they might be exploited as entry point for antibiotics.