Structural and Electrostatic *in silico* characterization of OmpF/OmpC orthologues

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In recent decades there was a drastic drop in the development of new antibiotics. This has increased the difficulty to counter the growing resistance to currently available antibiotics of many pathogens. Such a situation highlights the importance of developing alternative strategies aimed at looking for new scaffolds characterized by desired properties. The project of this work is to rationalize the transport of polar antibiotics and β-lactam inhibitors that exploit simple porins to penetrate the outer membrane of Gram-negative bacteria. Molecular Dynamics Simulations (MD) of porins and small molecules at an all-atom level allow investigating the physico-chemical parameters involved in their mutual interactions. We compared OmpF from *E. Coli* and its ortholog Omp35 from *Enterobacter Aerogenes*; OmpC from *E. Coli* and its ortologues Omp36 from *Enterobacter Aerogenes*, and OmpK36 from *Klabsiella Pneumoniae*.
Structural analysis of porins is the first step to understand how proteins interact with specific substrates and to find similarities between porins expressed by different species belonging to the same bacteria family: average cross section area along translocation axis and minimum area value were calculated from MD trajectory. Furthermore, MD Simulations allowed to compare distribution of charged residues and calculate the intrinsic electric field that might act as filter for dipolar molecules.

References

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