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Molecular dynamics simulations revealing the effect of the antimicrobial BP100 in phospholipidic bilayers

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Abstract: BP100, a short antimicrobial peptide, produces membrane perturbations that depend on lipid structure and charge, salts presence, and peptide/lipid molar ratios. As membrane perturbation mechanisms are not fully understood, the atomic scale nature of peptide/membrane interactions requires a close-up view analysis. Molecular Dynamics (MD) simulations are valuable tools for describing molecular interactions at the atomic level. In this work [1], we use MD simulations to investigate alterations in membrane properties consequent to BP100 binding to zwitterionic and anionic model membranes. We focused on membrane property changes upon peptide binding, namely membrane thickness, order parameters, surface curvature, lipid lateral diffusion and membrane hydration. In agreement with experimental results, our simulations showed that, when buried into the membrane, BP100 causes a decrease in lipid lateral diffusion and lipid acyl-chain order parameters and sharp local membrane thinning. These effects were most pronounced on the closest lipids in direct contact with the membrane-bound peptide. In DPPG and anionic-aggregate-containing DPPC/DPPG membranes, peptide flip (rotation of its non-polar facet towards the membrane interior) induced marked negative membrane curvature and enhanced the water residence half-life time in the lipid hydrophobic core and transmembrane water transport in the direction of the peptide. These results further elucidate the consequences of the initial interaction of cationic alpha-helical antimicrobial peptides with membranes.

Key-words: Molecular Dynamics, Atomistic simulations, Peptide, Membrane
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References:
[1] Leandro R. Franco, Peter Park, Hernan Chaimovich, Kaline Coutinho, Iolanda M. Cuccovia, Filipe S. Lima, RSC Adv., 12, (2022,) 4573–4588.