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Study of the antimicrobial peptide indolicidin and a mutant in micelle medium by molecular dynamics simulation

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ABSTRACT. The antimicrobial peptide indolicidin (IND) and the mutant CP10A in hydrated micelles were studied using molecular dynamics simulations in order to observe whether the molecular dynamics and experimental data could be sufficiently correlated and a detailed description of the interaction of the antimicrobial peptides with a model of the membrane provided by a hydrated micelle system could be obtained. In agreement with the experiments, the simulations showed that the peptides are located near the surface of the micelles. Peptide insertions agree with available experimental data, showing deeper insertion of the mutant compared with the peptide IND. Major insertion into the hydrophobic core of the micelle by all tryptophan and mutated residues of CP10A in relation to IND was observed. The charged residues of the terminus regions of both peptides present similar behavior, indicating that the major differences in the interactions with the micelles of the peptides IND and CP10A occur in the case of the hydrophobic residues.

Key words: Antimicrobial peptides; Indolicidin; Indolicidin mutant; Dodecylphosphocholine micelle; Peptide-micelle interaction; Molecular dynamics simulation

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