In Silico Analysis of Antimicrobial Peptides *Nicotiana alata* D1 and Human β Defensin-3: Sequence Alignment and Molecular Dynamics

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INTRODUCTION. Defensins, a class of antimicrobial peptides (AMPs) characterized by eight conserved cystein residues, these molecules and used by eukaryotes as a self-defense against pathogens. Defensins present an average molecular weight of 5 kDa and 45 to 54 amino acids and a Csαβ motif shape, which is structure are known by our antimicrobial activity. **OBJECTIVES:** Our aim to find which amino acid residues are conserved in defensins and evaluate the impact of their alteration in the peptide stability *in silico* using NaD1 (*Nicotiana alata* Defensin 1) and human's β Defensin-3 (HBD-3). **MATERIALS AND METHODS:** NaD1 and HBD-3 structures were recovered from PDB, then it was performed a sequence and structural alignment with 17 defensins to build a consensus logo sequence. After, it was studied the point mutations effects in the conserved residues. On this step the residues were modified and their structure submitted to a molecular dynamics simulations using GROMACS 5.0.5 and AMBER99SB-ILDN force field, during 10 nanoseconds. **DISCUSSION AND RESULTS**: Several conserved residues were found: eight cysteins, one acidic residue at position 27, three basic residues at positions 1, 39 and 40, one aromatic residue at position 10 and two glycines at positions 12 and 32. Analyzing the RMSD, radius of gyration and hydrogen bonds, the results show that none of the modifications caused any peptide denaturation during the simulation time, but the changes involving cysteins and glycines could promote the most significant alterations. **CONCLUSION:** The conserved residues, including the cysteins, are not essential to stabilize defensins fold (Csαβ motif), in addition there is evidence in the literature that they may be involved in the protection of the AMPs activity against bacterial proteases.

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