In Silico And Antimicrobial Analysis Of Three Analogs Peptides Derived From Native Peptide Stigmurin

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INTRODUCTION: From the transcriptome of the venom gland of the scorpion *Tityus stigmurus* it was identified an antimicrobial peptide (AMP) denominated Stigmurin, which have a primary structure of 17 amino acids and a net charge of +1. It was designed peptides analogs from this native peptide in order to potentialize its activity. OBJECTIVE: In the present study, we analyzed the structure and antibacterial activity of 3 analogs AMPs from Stigmurin. **MATERIAL AND METHODS**: We predicted the secondary structure, net charge and hydrofobic moment using PORTER and HeliQuest servers. Additionaly, it was performed computational modeling using I-tasser and AIDA, following solvatation using MDWeb, MolProbity was used to validate the obtained models. We conducted a screening of bacterial activity of the three synthetic peptides in *Escherichia coli* and two *Staphylococcus aureus* clinical strains, and the native peptide was used as control. Microorganisms incubated in Mueller Hinton broth were added the peptide in concentration of 0,25mg/ml or 0,50mg/ml, and bacterial growth was analyzed by microplate reader at 0, 18 and 24h at 595 nm. **RESULTS AND DISCUSSION**: In silico analysis reveals that two analogs peptides showed increased positive net charge, hydrophobic moment and α-helix structure compared with the native peptide. Whereas, the third analog peptide showed negative net charge, decrease in α-helix structure, and higher hydrofobic moment. In the antibacterial trials, the first two analogs have shown enhanced antimicrobial activity when compared to Stigmurin. This activity can be emphasized in *E. coli* strains, because Stigmurin showed no activity in this bacteria in all tests performed. Whilst, the third analog showed decrease in the antibacterial activity, that may be due to its negative charge and structure. **CONCLUSIONS**: Our work suggests that the positive charge, hydrophobic moment and α-helix strucutre may be related with encreased antimicrobial activity of AMPs. This enhanced activity potentiates the use of these molecules in pharmaceutical and food industry.

Palavras-Chaves: Antimicrobial peptide; Scorpion venom; Bioinformatics.
Patrocínio: CNPq, UFRN.