IDENTIFICATION AND STRUCTURAL INSIGHTS OF THREE NOVEL ANTIMICROBIAL PEPTIDES ISOLATED FROM GREEN COCONUT WATER

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Infections caused by pathogenic bacteria could cause an expressive negative impact on human health. A significant enhance in resistance to commercial antibiotics has been observed in all kinds of pathogenic bacteria. In order to find novel approaches to control such common infections, a wide number of defense peptides with bactericidal properties have been characterized. In this work, three peptides lower than 3 kDa were purified and identified from green coconut (*Cocos nucifera* L.) water by using reversed phase-high performance liquid chromatography (HPLC), showing molecular masses of 858 Da, 1249 Da and 950 Da. First one, named Cn-AMP1, was extremely efficient against both Gram-positive and Gram-negative bacteria, being MICs calculated for three peptides. All complete sequences were determined by MALDI-ToF analysis showing no identity in databanks. Moreover, peptide net charge and hydrophobicity of each peptide was *in silico* evaluated. Finally molecular modeling and dynamics were also applied generating peptides three-dimensional structures, indicating a better explanation to probable mechanisms of action. Cn-AMPs here reported show remarkable potential to contribute in the development of novel antibiotics from natural sources.

Keywords: antibacterial activity, green coconut water, antimicrobial peptides, mass spectrometry, *Cocos nucifera*.

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