Prospecting Antimicrobial Peptides from Medicinal Plants Using Bioinformatics Tools

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Antimicrobial peptides (AMPs) are biomolecules found in various living organisms. They are part of the natural defense of plants and have a broad spectrum of action against pathogens. The prospecting AMPs generally involves purification, characterization and functional assays methodologies, but in silico analyzes using only bioinformatics tools are promising. These analyzes are low-cost, easily accessible and have large-scale applicability to several molecules at the same time. Medicinal plants are good candidates for the study of natural compounds due to their therapeutic functions well documented in the literature. Many secondary metabolism compounds have antimicrobial activity, however, the antimicrobial proteins and peptides of these plants are little explored, despite their biotechnological potential. The objective of this work was to prospect AMPs from medicinal plants using in silico analysis for biotechnological applications. AMPs were investigated in four databases, NCBI-Protein, UniProtKB/Swiss-Prot, and the peptide-specific databases, APD3 and CAMP3. From the searches, 16 peptides from 8 different species of medicinal plants were selected to carry out in silico analyses. The peptide selection criterion was the structural and functional information available in the databases. Physicochemical analyzes were performed using Expasy software, toxicity prediction using ToxinPred software, protein/protein interaction using the STRING tool, toxicity prediction using iAMPpred and the subcellular localization of peptides was determined using CELLO v2.5. Physicochemical analyzes and toxicity prediction of peptides from 8 species of medicinal plants showed that 7 peptides do not present toxicity and have promising characteristics for biotechnological use. The protein-protein interaction results made it possible to discover and explore new functional molecules in the interaction network. Antimicrobial analyzes showed 5 peptides with a high probability of antibacterial activity. Furthermore, the cellular localization of the peptides was predicted, identifying 8 in the cytoplasm, 1 in the cell membrane and 7 in the extracellular space. This information is crucial for understanding the biological function and structural stability of antimicrobial peptides. The results identified peptides with a broad spectrum of antimicrobial activity and promising physicochemical characteristics, providing a selection of molecules for future in vitro explorations, including the rational design of new peptides.

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