Apoptosis Mediated by the Interaction Between Synthetic Peptides and the PAQR Receptor in Candida albicans: Discovery of a New Therapeutic Target of Clinical Interest

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Antibiotic resistance in recent decades has driven changes in the design and synthesis of new drugs. Promising candidates include synthetic peptides derived from osmotin proteins and plant thaumatin. The use of bioinformatics tools to identify antimicrobial peptides opens new possibilities for the development of potential drugs. The aim of this research was to search databases for osmotins to identify antimicrobial peptides through bioinformatics analysis, focusing on the probability and chemical parameters of these molecules. Additionally, molecular docking was performed to demonstrate the potential interactions of the peptides with the PAQR-type receptor located on the membrane of *Candida albicans.* Initially, a database search was conducted to find osmotins already recognized for their antimicrobial potential. The prediction of the three-dimensional structures of the best peptides found, as well as the PAQR membrane receptors in *Candida albicans*, was analyzed using the PEP-FOLD, GalaxyWEB, SWISS-MODEL, and AlphaFold programs. Molecular docking tests between three-dimensional peptide models and PAQR receptor models were carried out using the ClusPro 2.0 and HDOCK servers. The results from ClusPro and HDOCK were similar, suggesting that the peptides interact in two possible regions: the transmembrane region and the extracellular region. The OsmPep6 peptide interacted with the extracellular region of the PAQR receptor, forming 83 interactions, including 2 hydrogen bonds, with an HDOCK docking score of -175 kcal/mol and a confidence score of 0.60. Therefore, OsmPep6 has the potential to interact with the extracellular region of the PAQR-type receptor present in the *Candida albicans* membrane, potentially blocking the cellular function of this receptor. These results may contribute to the search for new therapeutic targets, providing insights into potential signaling mechanisms that trigger programmed cell death via the receptor.

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