

Title: MLAFP-XN: Leveraging neural network model for development of antifungal peptide identification tool

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Abstract: Infectious fungi have been an increasing global concern in the present era. A promising approach to tackle this pressing concern involves utilizing Antifungal peptides (AFP) to develop an antifungal drug that can selectively eliminate fungal pathogens from a host with minimal toxicity to the host. Accordingly, identifying precise therapeutic antifungal peptides is crucial for developing effective drugs and treatments. This study proposed MLAFP-XN, a neural network-based strategy for accurately detecting active AFP in sequencing data to achieve this objective. In this work, eight feature extraction techniques and the XGB feature selection strategy are utilized together to present an enhanced methodology. A total of 24 classification models were evaluated, and the most effective four have been selected. Each of these models demonstrated superior accuracy on independent test sets, with respective scores of 97.93 %, 99.47 %, and 99.48 %. Our model outperforms current state of the art methods. In addition, we created a companion website to demonstrate our AFP recognition process and use SHAP to identify the most influential properties.

Keywords: Antifungal peptide, Neural network, Antifungal drug, Feature extraction, Feature selection, Drug discovery

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