[BIOINFO 2023]

AMPs-GCN: Classification of antimicrobial peptide activites based on graph convolutional network

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Anti-microbial peptides (AMPs) have been found virtually in all organisms and are known to play crucial roles in innate immunity. They have gained attention as a substitute for antibiotics to address antibiotic resistance, and many efforts have been made to identify new AMPs. Various AMPs are identified to have at least one or more biological functions, including anti-bacterial, anti-fungal, and anti-viral activities. Existing classification models mainly utilize sequence information and physicochemical properties. Since biological activities are determined by their 3D structures, a model that learns the structural features of AMPs can lead to accurate functional classification. For this reason, we developed a multi-label classification model for AMPs using their structural features and graph convolutional network. A model was developed by utilizing predicted structures and sequence information using OmegaFold, which resulted in higher prediction performances when compared with existing models. The model demonstrated high performance in classifying not only between AMPs and non-AMPs but also in their functional activities. Utilization of the model can reduce the costs of screening and testing AMPs for developing therapeutics.