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GDAMP: Graph Neural Network for Antimicrobial Peptide Discovery with Enhanced Domain Sequence-level Interpretability

Hyeon Jun Yoon[1] and Minho Lee[1,*]

[1]*Department of Life Science, Dongguk University*
**Corresponding author: minholee@dgu.edu*

Antimicrobial peptides (AMPs), short natural-derived peptides, play a critical role in defending against diverse pathogenic microorganisms. Although many AI technologies have been developed for AMP screening, sequence-level information essential for protein function, such as domain and motif profiles, has rarely been directly incorporated. In this study, we propose GDAMP, a graph attention network designed for AMP discovery formulated as a classification task. GDAMP leverages domain and motif sequences identified by InterProScan and Motif—EmeRging and with Classes—Identification (MERCI). Protein sequences are preprocessed with ESM-2 embeddings and then fed into GDAMP, which performs sequence-level classification to distinguish AMPs from non-AMPs, and amino acid–level regression to estimate the probability of AMP-enriched domain distributions. Using the iAMPCN datasets, GDAMP achieved comparable or superior performance to state-of-the-art models. We further demonstrate its practical utility through case studies analyzing domain sequences with direct antimicrobial activity as well as indirect roles in enhancing host immunity.