Graduate School of Science and Technology Master's Thesis Abstract

Laboratory name (Supervisor)	Computational Systems Biologoy (Shigehiko Kanaya（Professor）)		
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Abstract

The increasing antimicrobial resistance (AMR) poses a significant global public health challenge, necessitating the discovery of new antibiotics to address this issue. This paper aims to explore a clustering-based approach utilizing deep learning techniques to predict the antimicrobial properties of natural products. We employ the K-means clustering algorithm and Information Maximizing Self-Augmented Training (IMSAT) to analyze the structural and chemical features of natural products, identifying potential drug candidates with latent antimicrobial activity. Through validation experiments, we demonstrate the effectiveness of the proposed method in predicting antimicrobial properties and present detailed experimental results. This research provides novel insights and tools to accelerate the discovery of new antibiotics and combat AMR.